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Statistical Analysis of Unreplicated Factorial Designs Using Contrasts

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STATISTICAL ANALYSIS OF UNREPLICATED FACTORIAL DESIGNS USING CONTRASTS

by

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(Under the Direction of Charles W. Champ)

ABSTRACT

Factorial designs can have a large number of treatments due to the number of factors and the number of levels of each factor. The number of experimental units required for a researcher to conduct a k factorial experiment is at least the number of treatments. For such an experiment, the total number of experimental units will also depend on the number of replicates for each treatment. The more experimental units used in a study the more the cost to the researcher. The minimum cost is associated with the case in which there is one experimental unit per treatment. That is, an unreplicated k factorial experiment would be the least costly. In an unreplicated experiment, the researcher cannot use analysis of variance to analyze the data. We propose a method that analyzes the data using normal probability plot of estimated contrast of the main effects and interactions. This method is applied to data and compared with Tukey's method that test for non-additivity. Our method is also discussed for use when the response is a multivariate set of measurements.

Key Words: Contrast, normal probability plot, factorial design, Tukey

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INTRODUCTION

Analyzing data from a designed experiment using ANalysis Of VAriance (ANOVA), generally requires at least two replicates for at least one treatment. There are, however, researchers who need to use unreplicated (one observation per treatment) designs. Under the independent normal model with common variance, these designs do not provide enough data to independently estimate the overall mean, main effects, interactions, and the common variance. Montgomery (1997) states concerning the analysis of data from an unreplicated two factor fixed effects design that "there are no tests on main effects unless the interaction effect is zero." He also points out that "even a moderate number of factors, the total number of treatment combinations in a 2^k factorial design is large." This is even a large number of total treatments for factorial designs in which the levels of one or more of the factors is greater than 2.

Three methods are discussed in the literature for analyzing the response data in a two factor fixed effects model with one observation per treatment. The first of these is to assume there is no interaction between the factors. This is the additive model. The second method uses a regression model that elimates higher-order polynomials. The third method is a test developed by Tukey (1949) for determining if there is an interaction. He states that "the professional practitioner of the analysis of variance will have no difficulty in extending the process to more complex designs." These methods are discussed in Alin and Kurt (2006) and Francka, Nielsenb, and Osbornec (2013). We will examine an extension of Tukey's method to a three factor design.

Various authors have examined method for evaluating the data from a 2^k factorial design with no replicates for a univariate response. One of these methods that is commonly recommended is the use of a normal probability plot of the estimates of the main effects and interactions. We plan to study the use of normal probability plots in the analysis of unreplicated k factorial designs in which each of the factors has two or more levels with at least one factor having three or more levels. This will include cases in which there is a univariate response and there is a multivariate response. As we will demonstrate, the estimators of the main effects and interactions in an unreplicated fixed effects k factor design in which at least one factor has more than two levels are correlated. We propose a transformation of these estimators to a collection of independent random variables with common variance. Under the hypothesis of no main effects or interactions, these estimators under the independent normal model with common variance σ^2 ($\boldsymbol{\Sigma}$ for a multivariate response) will be a random sample with common $N\left(0, \sigma^2\right)$ ($N_p\left(\mathbf{0}, \boldsymbol{\Sigma}\right)$ for a multivariate response) distributon. A normal probability plot of the transformed estimates of the main effects and interactions will be used to determine which linear combinations of the main effects and interactions are significantly different from zero. An examimation of the associated parameters will reveal which, if any, of the main effects and interactions are significantly different from zero.

CHAPTER 2

TWO FACTOR DESIGN MODEL WITH A UNIVARIATE RESPONSE

2.1 Introduction

In a variety of studies, researchers are interested in studying the effect of two or more factors on a response variable. As has been shown by a several authors, factorial designs are the most efficient way to conduct such studies. A factor is a variable whose values are selected by the researcher. The possible values of a factor are called the levels of the factor. How the values of a factor are selected determines if the study is a fixed effect or random effect factorial design. If the levels of a factor are the only ones of interest to the researcher, then the study is a fixed effect factorial design with respect this factor. If random selection is used to select from a collection of possible values of a factor the levels of the factor to be studied, then the factorial design is a random effects factorial design with respect to this factor. The treatments in a factorial design are all the possible factor level combinatins. In our study, it will be convenient to discuss first two-factor design with replications before examining designs without replicates.

2.2 The Two Factor Design with Replicates

We begin our study of factorial designs by examining two ($k = 2$) factor designs. Under the additive model, the response variable Y_{ijl} can be expressed as

$$Y_{ijl} = \mu_{ij} + \epsilon_{ijl}$$

with

$$\mu_{ij} = \mu + (\tau_1)_i + (\tau_2)_j + (\tau_{12})_{ij}$$

for $i = 1, \ldots, a$, $j = 1, \ldots, b$, and $l = 1, \ldots, n$ with $n > 1$. We have expressed the mean μ_{ij} of the response variable Y_{ijl} as the sum of an overall mean μ, the effect $(\tau_1)_i$ due to setting the first factor at level i, the effect $(\tau_2)_j$ of setting the second factor at its jth level, and an effect $(\tau_{12})_{ij}$ due to the interaction between the two factors when the first is set at its ith level and the second at its jth level. It is assumed that

$$\sum\nolimits_{i=1}^{a} (\tau_1)_i = 0; \sum\nolimits_{j=1}^{b} (\tau_2)_j = 0;$$
$$\sum\nolimits_{i=1}^{a} (\tau_{12})_{ij} = 0 \text{ for } j = 1, \ldots, b; \text{ and}$$
$$\sum\nolimits_{j=1}^{b} (\tau_{12})_{ij} = 0 \text{ for } i = 1, \ldots, a.$$

We also assume that the Y_{ijl}'s are independent and $\epsilon_{ijl} \sim N\left(0, \sigma_{ij}^2\right)$. We refer to these assumptions as the independent normal model. The model is further simplified by assuming a common variance, that is, $\sigma_{ijl}^2 = \sigma^2$ the common variance for $i = 1, \ldots, a$, $j = 1, \ldots, b$, and $l = 1, \ldots, n$. The design is an unreplicated one if $n = 1$. Using matrix notation, we can write our additive model in the form

$$\mathbf{Y} = \mathbf{X}\theta + \epsilon,$$

where $\mathbf{Y}$ is the $abn \times 1$ vector of observations, $\mathbf{X}$ is the $abn \times ab$ design matrix, θ is the $ab \times 1$ vector of model parameters, and ϵ is the $abn \times 1$ vector of error terms.

An analysis of variance (ANOVA) of the response data is based on the following partition of the sum of squares total (SST).

$$SST = SSA + SSB + SSAB + SSE,$$

where

$$SST = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{l=1}^{n} \left(Y_{ijl} - \overline{Y}_{...}\right)^2;$$
$$SSA = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{l=1}^{n} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2;$$
$$SSB = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{l=1}^{n} \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2;$$
$$SSAB = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{l=1}^{n} \left(\overline{Y}_{ij.} - \overline{Y}_{i..} - \overline{Y}_{.j.} + \overline{Y}_{...}\right)^2; \text{ and}$$
$$SSE = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{l=1}^{n} \epsilon_{ijl}^2.$$

It can be shown that SSA, SSB, $SSAB$, and SSE are stochastically independent under our independent normal model. The degrees of freedom of these sums of squares are

$$df_{SST} = abn - 1;\ df_{SSA} = a - 1;\ df_{SSB} = b - 1;$$
$$df_{SSAB} = (a-1)(b-1);\ \text{and } df_{SSE} = (n-1)\,ab.$$

The mean squares associated with SSA, SSB, $SSAB$, and SSE are, respectively,

$$MSA = \frac{SSA}{df_{SSA}},\ MSB = \frac{SSB}{df_{SSB}},\ MSAB = \frac{SSAB}{df_{SSAB}},\ \text{and } MSE = \frac{SSE}{df_{SSE}}.$$

Note that if $n = 1$, then $df_{SSE} = 0$ and the MSE is undefined.

The null (H_0) and alternative (H_1) hypotheses of interest can be written in terms of the following hypotheses.

$$H_{A,0} : (\tau_1)_1 = \ldots = (\tau_1)_a = 0 \text{ and } H_{A,1} :\sim H_{A,0};$$
$$H_{B,0} : (\tau_2)_1 = \ldots = (\tau_2)_b = 0 \text{ and } H_{B,1} :\sim H_{B,0}; \text{ and}$$
$$H_{AB,0} : (\tau_{12})_{11} = \ldots = (\tau_{12})_{ab} = 0 \text{ and } H_{AB,1} :\sim H_{AB,0}$$

The alternative hypothesis in this study is

$$H_1 : H_{AB,1} \vee [H_{AB,0} \wedge (H_{A,1} \vee H_{B,1})]$$

with the null hypothesis

$$H_0 :\sim H_1.$$

The statistical test has decision rule that rejects the null hypotheis in favor of the alternative hypothesis if the observed value of

$$\frac{MSAB}{MSE} \geq c_{AB} \vee \left[\frac{MSAB}{MSE} < c_{AB} \wedge \left(\frac{MSA}{MSE} \geq c_A \vee \frac{MSB}{MSE} \geq c_B\right)\right].$$

It can be shown that

$$\frac{SSA}{\sigma^2} \sim \chi^2_{a-1,\xi_A^2}, \ \frac{SSB}{\sigma^2} \sim \chi^2_{b-1,\xi_B^2}, \ \frac{SSAB}{\sigma^2} \sim \chi^2_{(a-1)(b-1),\xi_{AB}^2}, \text{ and } \frac{SSE}{\sigma^2} \sim \chi^2_{(n-1)ab},$$

where

$$\xi_A^2 = \frac{nb\sum_{i=1}^{a}(\tau_1)_i^2}{a\sigma^2}, \ \xi_B^2 = \frac{na\sum_{j=1}^{b}(\tau_2)_j^2}{b\sigma^2}, \text{ and } \xi_{AB}^2 = \frac{n\sum_{i=1}^{a}\sum_{j=1}^{b}(\tau_{12})_{ij}^2}{\sigma^2\left[(a-1)(b-1)+1\right]}.$$

If the null hypothesis is true, then we have $\xi_A = \xi_B = \xi_{AB} = 0$. The size of the test α is given by

$$\begin{aligned}
\alpha &= P\left(\frac{MSAB}{MSE} \geq c_{AB} \vee \left[\frac{MSAB}{MSE} < c_{AB} \wedge \left(\frac{MSA}{MSE} \geq c_A \vee \frac{MSB}{MSE} \geq c_B\right)\right]\right) \\
&= P\left(\frac{\chi^2_{(a-1)(b-1)}/\left[(a-1)(b-1)\right]}{\chi^2_{(n-1)ab}/\left[(n-1)ab\right]} \geq c_{AB}\right) \\
&+ P\left(\frac{\chi^2_{(a-1)(b-1)}/\left[(a-1)(b-1)\right]}{\chi^2_{(n-1)ab}/\left[(n-1)ab\right]} < c_{AB}, \frac{\chi^2_{a-1}/(a-1)}{\chi^2_{(n-1)ab}/\left[(n-1)ab\right]} \geq c_A\right) \\
&+ P\left(\frac{\chi^2_{(a-1)(b-1)}/\left[(a-1)(b-1)\right]}{\chi^2_{(n-1)ab}/\left[(n-1)ab\right]} < c_{AB}, \frac{\chi^2_{b-1}/(b-1)}{\chi^2_{(n-1)ab}/\left[(n-1)ab\right]} \geq c_B\right) \\
&= 1 - F_{F_{(a-1)(b-1),(n-1)ab}}(c_{AB}) \\
&+ \int_0^\infty F_{\chi^2_{(a-1)(b-1)}}\left(\frac{(n-1)abxc_{AB}}{(a-1)(b-1)}\right)\overline{F}_{\chi^2_{a-1}}\left(\frac{(n-1)abxc_A}{a-1}\right)f_{\chi^2_{(n-1)ab}}(x)\,dx \\
&+ \int_0^\infty F_{\chi^2_{(a-1)(b-1)}}\left(\frac{(n-1)abxc_{AB}}{(a-1)(b-1)}\right)\overline{F}_{\chi^2_{b-1}}\left(\frac{(n-1)abxc_B}{b-1}\right)f_{\chi^2_{(n-1)ab}}(x)\,dx,
\end{aligned}$$

where

$$\overline{F}_{\chi^2_{a-1}}\left(\frac{(n-1)\,abxc_A}{a-1}\right) = 1 - F_{\chi^2_{a-1}}\left(\frac{(n-1)\,abxc_A}{a-1}\right) \text{ and}$$
$$\overline{F}_{\chi^2_{b-1}}\left(\frac{(n-1)\,abxc_B}{b-1}\right) = 1 - F_{\chi^2_{b-1}}\left(\frac{(n-1)\,abxc_B}{b-1}\right).$$

The power of the test is determined by

$$\begin{aligned} power = 1 &- F_{F_{(a-1)(b-1),m-ab,\xi_{AB}}}(c_{AB}) \\ &+ \int_0^\infty F_{\chi^2_{(a-1)(b-1),\xi_{AB}}}\left(\frac{(m-ab)\,xc_{AB}}{(a-1)(b-1)}\right)\left[1 - F_{\chi^2_{a-1,\xi_A}}\left(\frac{(m-ab)\,xc_A}{a-1}\right)\right] f_{\chi^2_{m-ab}}(x)\,dx \\ &+ \int_0^\infty F_{\chi^2_{(a-1)(b-1),\xi_{AB}}}\left(\frac{(m-ab)\,xc_{AB}}{(a-1)(b-1)}\right)\left[1 - F_{\chi^2_{b-1,\xi_B}}\left(\frac{(m-ab)\,xc_B}{b-1}\right)\right] f_{\chi^2_{m-ab}}(x)\,dx, \end{aligned}$$

where at least one of the value ξ_A, ξ_B, and ξ_{AB} is not equal to zero.

2.3 One Observation per Treatment No Interaction Assumed

For the case of one observation per treatment ($n = 1$), there is only enough data to estimate independently the overall mean, the main effects, and the interactions but not the common variance in our model. One approach to analyzing the data for main effects is to assume there is no interaction between the two factors. In this case the model becomes

$$\mu_{ij} = \mu + (\tau_1)_i + (\tau_2)_j\,.$$

The null and alternative hypotheses are

$$H_0 : (\tau_1)_1 = \ldots = (\tau_1)_a = 0 \text{ and } (\tau_2)_1 = \ldots = (\tau_2)_b = 0; \text{ and}$$
$$H_1 :\sim H_0.$$

The total sum of squares (SST) can be partitioned into the sum of square due to the first factor (SSA), the sum of squares due to the second factor (SSB), and the sum of squares (SSE) due to error. That is,

$$SST = SSA + SSB + SSE.$$

There respective degrees of freedom are

$$df_{SST} = ab - 1,\ df_{SSA} = a - 1,\ df_{SSB} = b - 1, \text{ and } df_{SSE} = (a-1)(b-1).$$

Under this model, it can be shown that

$$\frac{SSA}{\sigma^2} \sim \chi^2_{a-1,\xi_A^2},\ \frac{SSB}{\sigma^2} \sim \chi^2_{b-1,\xi_B^2}, \text{ and } \frac{SSE}{\sigma^2} \sim \chi^2_{(n-1)ab},$$

where

$$\xi_A^2 = \frac{nb\sum_{i=1}^{a}(\tau_1)_i^2}{a\sigma^2}, \text{ and } \xi_B^2 = \frac{na\sum_{j=1}^{b}(\tau_2)_j^2}{b\sigma^2}.$$

The test based on the analysis of variances rejects H_0 in favor of H_1 if the observed value of

$$\frac{MSA}{MSE} \geq c_A \vee \frac{MSB}{MSE} \geq c_B,$$

where

$$\begin{aligned} MSA &= \frac{b\sum_{i=1}^{a}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)^2}{a-1},\ MSB = \frac{a\sum_{j=1}^{b}\left(\overline{Y}_{.j} - \overline{Y}_{..}\right)^2}{b-1}, \text{ and} \\ MSE &= \frac{SST - SSA - SSB}{(a-1)(b-1)}. \end{aligned}$$

The size of the test is

$$\begin{aligned} \alpha &= P\left(\frac{MSA}{MSE} \geq c_A\right) + P\left(\frac{MSB}{MSE} \geq c_B\right) - P\left(\frac{MSA}{MSE} \geq c_A\right) P\left(\frac{MSB}{MSE} \geq c_B\right) \\ &= P\left(F_{a-1,(a-1)(b-1)} \geq c_A\right) + P\left(F_{b-1,(a-1)(b-1)} \geq c_B\right) \\ &- \int_0^\infty P\left(\chi^2_{a-1} \geq \frac{xc_A}{b-1}\right) P\left(\chi^2_{b-1} \geq \frac{xc_B}{a-1}\right) f_{\chi^2_{(a-1)(b-1)}}(x)\, dx \\ &= 1 - F_{F_{a-1,(a-1)(b-1)}}(c_A) + 1 - F_{F_{b-1,(a-1)(b-1)}}(c_B) \\ &- \int_0^\infty \overline{F}_{\chi^2_{a-1}}\left(\frac{xc_A}{b-1}\right) \overline{F}_{\chi^2_{b-1}}\left(\frac{xc_B}{a-1}\right) f_{\chi^2_{(a-1)(b-1)}}(x)\, dx, \end{aligned}$$

where

$$\overline{F}_{\chi^2_{a-1}}\left(\frac{xc_A}{b-1}\right)=1-F_{\chi^2_{a-1}}\left(\frac{xc_A}{b-1}\right) \text{ and } \overline{F}_{\chi^2_{b-1}}\left(\frac{xc_B}{a-1}\right)=1-F_{\chi^2_{b-1}}\left(\frac{xc_B}{a-1}\right).$$

For example in the case in which $a = 3$ and $b = 5$, if the researcher selects the critical values c_A and c_B to be

$$c_A = F_{3-1,(3-1)(5-1),0.05} \text{ and } c_B = F_{5-1,(3-1)(5-1),0,05},$$

then the actual size of the test is

$$\begin{aligned}
\alpha &= 2\alpha - \int_0^{\infty}\left(1-\text{ChiSquareDist}\left(\frac{x\text{FInv}\left(1-\alpha; a-1, (a-1)(b-1)\right)}{b-1}; a-1\right)\right) \\
&\quad \times\left(1-\text{ChiSquareDist}\left(\frac{x\text{FInv}\left(1-\alpha; b-1, (a-1)(b-1)\right)}{a-1}; a-1\right)\right) \\
&\quad \times\text{ChiSquareDen}\left(x; (a-1)(b-1)\right)dx \\
&= 0.0962225486\underline{3}.
\end{aligned}$$

2.4 Tukey's Method for One Observation per Treatment

Tukey (1949) developed a test for determining if there is an interaction between the two factors which assumes the interactions are of the form

$$(\tau_{12})_{ij} = \lambda\,(\tau_1)_i\,(\tau_2)_j\,.$$

In this model, the $a + b + 2$ parameters including the common variance can be estimated. To determine these estimates using least squares we define the function

$$\begin{aligned}
Q &= Q\left(\mu, (\tau_1)_1, \ldots, (\tau_1)_a, (\tau_2)_1, \ldots, (\tau_2)_b, \lambda\right) \\
&= \sum\nolimits_{i=1}^{a}\sum\nolimits_{j=1}^{b}\left(Y_{ij}-\mu-(\tau_1)_i-(\tau_2)_j-\lambda\,(\tau_1)_i\,(\tau_2)_j\right)^2
\end{aligned}$$

The least square estimates are the solutions to the following system of equations.

$$\frac{\partial Q}{\partial\mu}=0;\ \frac{\partial Q}{\partial(\tau_1)_i}=0;\ \frac{\partial Q}{\partial(\tau_2)_j}=0;\ \frac{\partial Q}{\partial\lambda}=0.$$

The least squares estimates of the parameters μ, $(\tau_1)_1$, ..., $(\tau_1)_a$, $(\tau_2)_1$,...,$(\tau_2)_b$, and λ are given, respectively, by

$$\widehat{\mu} = \overline{Y}_{..},\ (\widehat{\tau}_1)_i = \overline{Y}_{i.} - \overline{Y}_{..},\ (\widehat{\tau}_2)_j = \overline{Y}_{.j} - \overline{Y}_{..}, \text{ and}$$
$$\widehat{\lambda} = \frac{\sum_{i=1}^{a}\sum_{j=1}^{b}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)\left(\overline{Y}_{.j} - \overline{Y}_{..}\right)Y_{ij}}{\sum_{i=1}^{a}\sum_{j=1}^{b}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)^2\left(\overline{Y}_{.j} - \overline{Y}_{..}\right)^2}.$$

We can now express Y_{ij} as

$$Y_{ij} = \overline{Y}_{..} + \left(\overline{Y}_{i.} - \overline{Y}_{..}\right) + \left(\overline{Y}_{.j} - \overline{Y}_{..}\right) + \widehat{\lambda}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)\left(\overline{Y}_{.j} - \overline{Y}_{..}\right) + \widehat{\epsilon}_{ij}.$$

It follows that $\widehat{\epsilon}_{ij}$ can be expressed as

$$\widehat{\epsilon}_{ij} = Y_{ij} - \overline{Y}_{..} - \left(\overline{Y}_{i.} - \overline{Y}_{..}\right) - \left(\overline{Y}_{.j} - \overline{Y}_{..}\right) - \widehat{\lambda}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)\left(\overline{Y}_{.j} - \overline{Y}_{..}\right).$$

The total sum of squares SST can now be partitioned into

$$SST = SSA + SSB + SSAB^* + SSE^*,$$

where SST, SSA, and SSB are defined in the previous section with

$$SSAB^* = \sum_{i=1}^{a}\sum_{j=1}^{b}\widehat{\lambda}^2\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)^2\left(\overline{Y}_{.j} - \overline{Y}_{..}\right)^2 \text{ and}$$
$$SSE^* = \sum_{i=1}^{a}\sum_{j=1}^{b}\widehat{\epsilon}_{ij}^2.$$

The degrees of freedom of $SSAB^*$ and SSE^* are, respectively, 1 and $ab - a - b$. It can be shown that under $H_0 : \lambda = 0$, the random variables $SSAB^*$ and SSE^* are stochastically independent with

$$\frac{SSAB^*}{\sigma^2} \sim \chi_1^2 \text{ and } \frac{SSE^*}{\sigma^2} \sim \chi_{ab-a-b}^2.$$

The appropriate hypotheses in this case are

$$H_0 :\sim H_1 \text{ with } H_1 : H_{\lambda,1} \vee \left[H_{\lambda,0} \wedge \left(H_{A,1} \vee H_{B,1}\right)\right],$$

where

$$H_{\lambda,0} : \lambda = 0 \text{ and } H_{\lambda,1} : \lambda \neq 0.$$

The statistical test has decision rule that rejects the null hypotheis in favor of the alternative hypothesis if the observed value of

$$\frac{MSAB^*}{MSE^*} \geq c_{AB} \vee \left[\frac{MSAB^*}{MSE^*} < c_{AB} \wedge \left(\frac{MSA}{MSE^*} \geq c_A \vee \frac{MSB}{MSE^*} \geq c_B\right)\right],$$

where

$$MSAB^* = \frac{SSAB^*}{1} \text{ and } MSE^* = \frac{SSE^*}{ab-a-b}.$$

The size of the test α is

$$\alpha = 1 - F_{F_{1,ab-a-b}}\left(c_{AB}\right) + \int_0^\infty F_{\chi_1^2}\left(\frac{xc_{AB}}{ab-a-b}\right) \overline{F}_{\chi_{a-1}^2}\left(\frac{(a-1)\,xc_A}{ab-a-b}\right) f_{\chi_{ab-a-b}^2}(x)\,dx$$
$$+ \int_0^\infty F_{\chi_1^2}\left(\frac{xc_{AB}}{ab-a-b}\right) \overline{F}_{\chi_{b-1}^2}\left(\frac{(b-1)\,xc_B}{ab-a-b}\right) f_{\chi_{ab-a-b}^2}(x)\,dx.$$

2.5 Using a Normal Probability Plot

The least squares estimate $\widehat{\theta}$ of the vector of parameters θ in the full model with no replicates is

$$\widehat{\theta} = \left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{Y}.$$

It can be shown that if $a > 2$, then the estimators $\left(\widehat{\tau}_1\right)_1, \ldots, \left(\widehat{\tau}_1\right)_{a-1}$ of the parameters $\left(\tau_1\right)_1, \ldots, \left(\tau_1\right)_{a-1}$ are not independent under our independent normal model. Likewise, if $b > 2$, the estimators $\left(\widehat{\tau}_2\right)_1, \ldots, \left(\widehat{\tau}_2\right)_{b-1}$ of the parameters $\left(\tau_2\right)_1, \ldots, \left(\tau_2\right)_{b-1}$ are not stochastically independent as are the estimators $\left(\widehat{\tau}_{12}\right)_{ij}$ of the parameters $\left(\tau_{12}\right)_{ij}$ when $a > 2$ and/or $b > 2$. This can be seen by first noting that

$$\mathbf{\Sigma}_{\widehat{\theta}} = cov\left(\widehat{\theta}\right) = \left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}\sigma^2$$

and observing that $\left(\mathbf{X^TX}\right)^{-1}$ is not the identity matrix. However, it can be shown that $\left(\mathbf{X^TX}\right)^{-1}$ has the form

$$\left(\mathbf{X^TX}\right)^{-1} = \begin{bmatrix} w & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{W}_A^{(a-1)\times(a-1)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W}_B^{(b-1)\times(b-1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{W}_{AB}^{(a-1)(b-1)\times(a-1)(b-1)} \end{bmatrix},$$

where w corresponds to the overall mean, $\mathbf{W}_A^{(a-1)\times(a-1)}$ is associated with the main effects due to factor A, $\mathbf{W}_B^{(b-1)\times(b-1)}$ is associated with the main effects due to factor B, and $\mathbf{W}_{AB}^{(a-1)(b-1)\times(a-1)(b-1)}$ is associated with the interactions between factors A and B. We can now see that, for example,

$$cov\left(\left(\widehat{\tau}_1\right)\right) = \mathbf{W}_A^{(a-1)\times(a-1)}\sigma^2$$

whereas

$$cov\left(\left(\widehat{\tau}_1, \widehat{\tau}_2\right)\right) = \mathbf{0},$$

where

$$\widehat{\tau}_1 = \left[\left(\widehat{\tau}_1\right)_1, \ldots, \left(\widehat{\tau}_1\right)_{a-1}\right]^{\mathbf{T}} \text{ and } \widehat{\tau}_2 = \left[\left(\widehat{\tau}_2\right)_1, \ldots, \left(\widehat{\tau}_2\right)_{b-1}\right]^{\mathbf{T}}.$$

Observe that $\left(\mathbf{X^TX}\right)^{-1}$ is a real symmetric matrix. In particular, observe that $\mathbf{W}_A$, $\mathbf{W}_B$, and $\mathbf{W}_{AB}$ are real symmetric matrices. It follows that there exist matrices $\mathbf{P}_A$, $\mathbf{P}_B$, and $\mathbf{P}_{AB}$ such that

$$\mathbf{W}_A = \mathbf{P}_A\mathbf{P}_A^{\mathbf{T}},\ \mathbf{W}_B = \mathbf{P}_B\mathbf{P}_B^{\mathbf{T}}, \text{ and } \mathbf{W}_{AB} = \mathbf{P}_{AB}\mathbf{P}_{AB}^{\mathbf{T}}.$$

We define $\mathbf{P}$ by

$$\mathbf{P} = \begin{bmatrix} \sqrt{w} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{P}_A & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{P}_B & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{P}_{AB} \end{bmatrix}.$$

It follows that the vector of transformed estimators $\widehat{\theta}^*$ define by

$$\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta}$$

are stochastically independent since

$$\mathbf{\Sigma}_{\widehat{\theta}^*} = cov\left(\mathbf{P}^{-1}\widehat{\theta}\right) = \mathbf{P}^{-1}\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}\left(\mathbf{P}^{-1}\right)^{\mathbf{T}}\sigma^2 = \mathbf{I}\sigma^2.$$

The vector estimator $\widehat{\theta}^*$ is associated with the contrast given in $\mathbf{W}_A$, $\mathbf{W}_B$, and $\mathbf{W}_{AB}$ of the vector of parameters θ. This suggest that under our null hypothesis of no main effects or interactions that the estimators

$$\widehat{\theta}_2^*, \ldots, \widehat{\theta}_{(a-1)(b-1)}^*$$

are stochastically independent and identically distributed $N\left(0, \sigma^2\right)$. A normal probability plot of the observed values of these estimators should reveal which if any of these linear combinations of the estimators of the main effects and interactions are different from zero. Exact plotting positions for a normal probability plot can be found in Harter (1961) and Teichroew (1956) for selected values of the sample size. Often the ith plotting position $E\left(Z_{i:n}\right)$ for a normal probability plot is usually approximated by

$$E\left(Z_{i:n}\right) = \Phi^{-1}\left(\frac{i - 0.375}{n + 0.25}\right),$$

where $Z_{i:n}$ is the ith order statistics of a random sample of size n from a standard normal distribution and $\Phi\left(z\right)$ is the cumulative distribution function of a standard normal distribution. This approximation was originally proposed by Blom (1958). A discussion on the selection of plotting positions are discussed in Champ and Vora (2005).

2.6 Some Examples

Example 1:

Montgomery (1997) gives an example of a two factor experiment in which $n_{ij} = 1$ for $i = 1, 2, 3$ and $j = 1, 2, 3, 4, 5$. He states in his Example 6-2 that the "impurity present in a chemical product is affected by two factors – presure and temperature." His data is presented in the following table.

Table 2.1: Montgomery's Example 6-2

		Temperature				
		25	30	35	40	45
	100	5	4	6	3	5
Pressure	125	3	1	4	2	3
	150	1	1	3	1	2

Using Tukey's method, he conclude that there was no interaction effect but that the main effects due to both temperature and pressure are significant.

The design matrix for this experiment is

$$\mathbf{X} = \begin{bmatrix}
1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\
1 & -1 & -1 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
1 & -1 & -1 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 \\
1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 \\
1 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 \\
1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}.$$

It follows that

$$w = \frac{1}{15},\ \mathbf{W}_A = \begin{bmatrix} \frac{2}{15} & -\frac{1}{15} \\ -\frac{1}{15} & \frac{2}{15} \end{bmatrix},$$

$$\mathbf{W}_B = \begin{bmatrix} \frac{4}{15} & -\frac{1}{15} & -\frac{1}{15} & -\frac{1}{15} \\ -\frac{1}{15} & \frac{4}{15} & -\frac{1}{15} & -\frac{1}{15} \\ -\frac{1}{15} & -\frac{1}{15} & \frac{4}{15} & -\frac{1}{15} \\ -\frac{1}{15} & -\frac{1}{15} & -\frac{1}{15} & \frac{4}{15} \end{bmatrix}, \text{ and}$$

$$\mathbf{W}_{AB} = \begin{bmatrix} \frac{8}{15} & -\frac{2}{15} & -\frac{2}{15} & -\frac{2}{15} & -\frac{4}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} \\ -\frac{2}{15} & \frac{8}{15} & -\frac{2}{15} & -\frac{2}{15} & \frac{1}{15} & -\frac{4}{15} & \frac{1}{15} & \frac{1}{15} \\ -\frac{2}{15} & -\frac{2}{15} & \frac{8}{15} & -\frac{2}{15} & \frac{1}{15} & \frac{1}{15} & -\frac{4}{15} & \frac{1}{15} \\ -\frac{2}{15} & -\frac{2}{15} & -\frac{2}{15} & \frac{8}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & -\frac{4}{15} \\ -\frac{4}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{8}{15} & -\frac{2}{15} & -\frac{2}{15} & -\frac{2}{15} \\ \frac{1}{15} & -\frac{4}{15} & \frac{1}{15} & \frac{1}{15} & -\frac{2}{15} & \frac{8}{15} & -\frac{2}{15} & -\frac{2}{15} \\ \frac{1}{15} & \frac{1}{15} & -\frac{4}{15} & \frac{1}{15} & -\frac{2}{15} & -\frac{2}{15} & \frac{8}{15} & -\frac{2}{15} \\ \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & -\frac{4}{15} & -\frac{2}{15} & -\frac{2}{15} & -\frac{2}{15} & \frac{8}{15} \end{bmatrix}.$$

It can be shown

$$\mathbf{P}_A = \begin{bmatrix} \frac{\sqrt{30}}{30} & \frac{\sqrt{10}}{10} \\ \frac{\sqrt{30}}{30} & -\frac{\sqrt{10}}{10} \end{bmatrix},$$

$$\mathbf{P}_B = \begin{bmatrix} \frac{\sqrt{15}}{30} & \frac{\sqrt{6}}{6} & \frac{\sqrt{18}}{18} & \frac{1}{6} \\ \frac{\sqrt{15}}{30} & 0 & 0 & -\frac{3}{6} \\ \frac{\sqrt{15}}{30} & 0 & -\frac{2\sqrt{18}}{18} & \frac{1}{6} \\ \frac{\sqrt{15}}{30} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{18}}{18} & \frac{1}{6} \end{bmatrix}, \text{ and}$$

$$\mathbf{P}_{AB} = \begin{bmatrix} \frac{\sqrt{30}}{60} & \frac{\sqrt{10}}{20} & \frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{\sqrt{2}}{12} & \frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{12} \\ \frac{\sqrt{30}}{60} & \frac{\sqrt{10}}{20} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{6}}{4} \\ \frac{\sqrt{30}}{60} & \frac{\sqrt{10}}{20} & 0 & -\frac{1}{3} & \frac{\sqrt{2}}{12} & 0 & -\frac{\sqrt{3}}{3} & \frac{\sqrt{6}}{12} \\ \frac{\sqrt{30}}{60} & \frac{\sqrt{10}}{20} & -\frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{\sqrt{2}}{12} & -\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{12} \\ \frac{\sqrt{30}}{60} & -\frac{\sqrt{10}}{20} & \frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{\sqrt{2}}{12} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{12} \\ \frac{\sqrt{30}}{60} & -\frac{\sqrt{10}}{20} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{6}}{4} \\ \frac{\sqrt{30}}{60} & -\frac{\sqrt{10}}{20} & 0 & -\frac{1}{3} & \frac{\sqrt{2}}{12} & 0 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{6}}{12} \\ \frac{\sqrt{30}}{60} & -\frac{\sqrt{10}}{20} & -\frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{\sqrt{2}}{12} & \frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{12} \end{bmatrix}.$$

We observe that our least squares estimates are

$$\begin{aligned} \widehat{\theta} &= \left(\mathbf{X^T X}\right)^{-1} \mathbf{X^T y} \\ &= \begin{bmatrix} \frac{44}{15} & \frac{5}{3} & -\frac{1}{3} & \frac{1}{15} & -\frac{14}{15} & \frac{7}{5} & -\frac{14}{15} & \frac{1}{3} & \frac{1}{3} & 0 & -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} & 0 & \frac{1}{3} \end{bmatrix}^{\mathbf{T}}, \end{aligned}$$

where

$$\mathbf{y} = \begin{bmatrix} 5 & 4 & 6 & 3 & 5 & 3 & 1 & 4 & 2 & 3 & 1 & 1 & 3 & 1 & 2 \end{bmatrix}^{\mathbf{T}}.$$

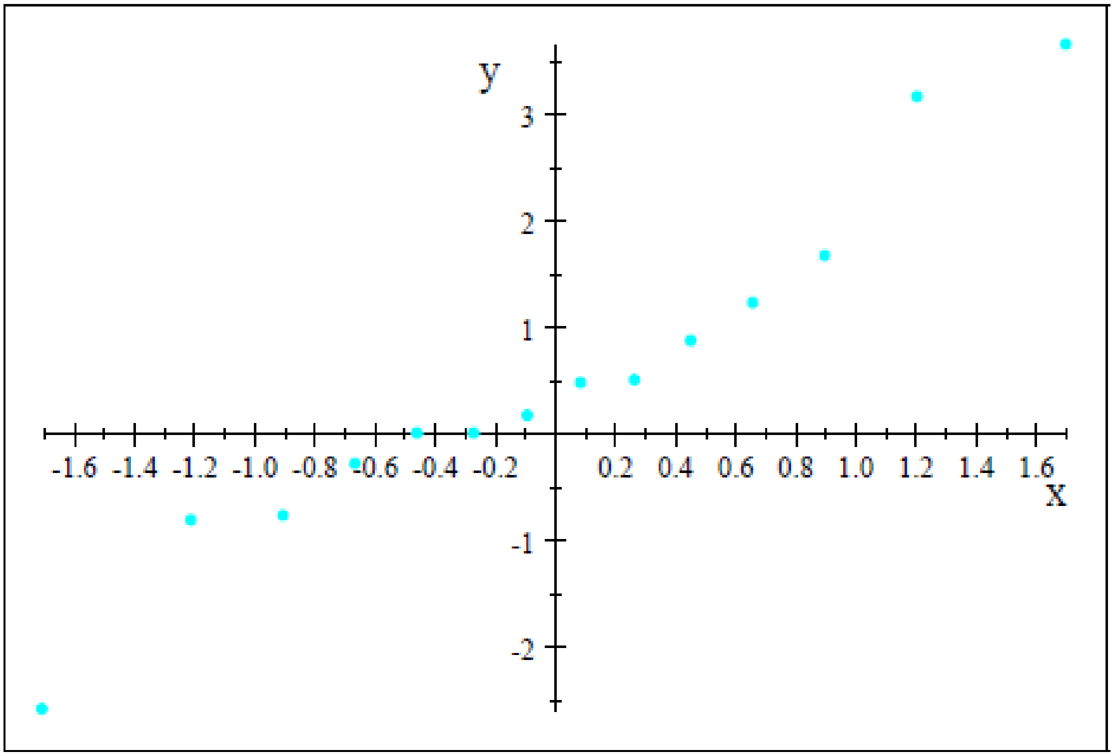
It then follows that

$$\begin{aligned} \widehat{\theta}^* &= \mathbf{P}^{-1}\widehat{\theta} \\ &= \begin{bmatrix} \frac{44\sqrt{15}}{15} & \frac{2\sqrt{30}}{3} & \sqrt{10} & -\frac{\sqrt{15}}{5} & \frac{\sqrt{6}}{2} & -\frac{11\sqrt{2}}{6} & \frac{5}{3} & 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{6} & \frac{\sqrt{2}}{3} & \frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{3} \end{bmatrix}^{\mathbf{T}}. \end{aligned}$$

Omitting the estimate for $\mu^* = 44\sqrt{15}/15$, we find the observed order statistics for the remaining fourteen contrast estimates. From Teicherow (1956), we obtain the plotting position for a normal probability plot for a sample size of fourteen. These ordered pairs are given in the following 14×2 matrix with the plotting position in the first column and the ordered data in the second.

$$\begin{bmatrix} -1.7033815541 & -\frac{11\sqrt{2}}{6} \\ -1.2079022754 & -\frac{\sqrt{6}}{3} \\ -0.9011267039 & -\frac{\sqrt{15}}{5} \\ -0.6617637035 & -\frac{\sqrt{3}}{6} \\ -0.4555660500 & 0 \\ -0.2672970489 & 0 \\ -0.0881592141 & \frac{1}{6} \\ 0.0881592141 & \frac{\sqrt{2}}{3} \\ 0.2672970489 & \frac{1}{2} \\ 0.4555660500 & \frac{\sqrt{3}}{2} \\ 0.6617637035 & \frac{\sqrt{6}}{2} \\ 0.9011267039 & \frac{5}{3} \\ 1.2079022754 & \sqrt{10} \\ 1.7033815541 & \frac{2\sqrt{30}}{3} \end{bmatrix}$$

Figure 2.1: Montgomery Example, Probability Plot



This plots suggest that eleven of the points are plotting about a line whereas three are not plotting about this line. These are the points

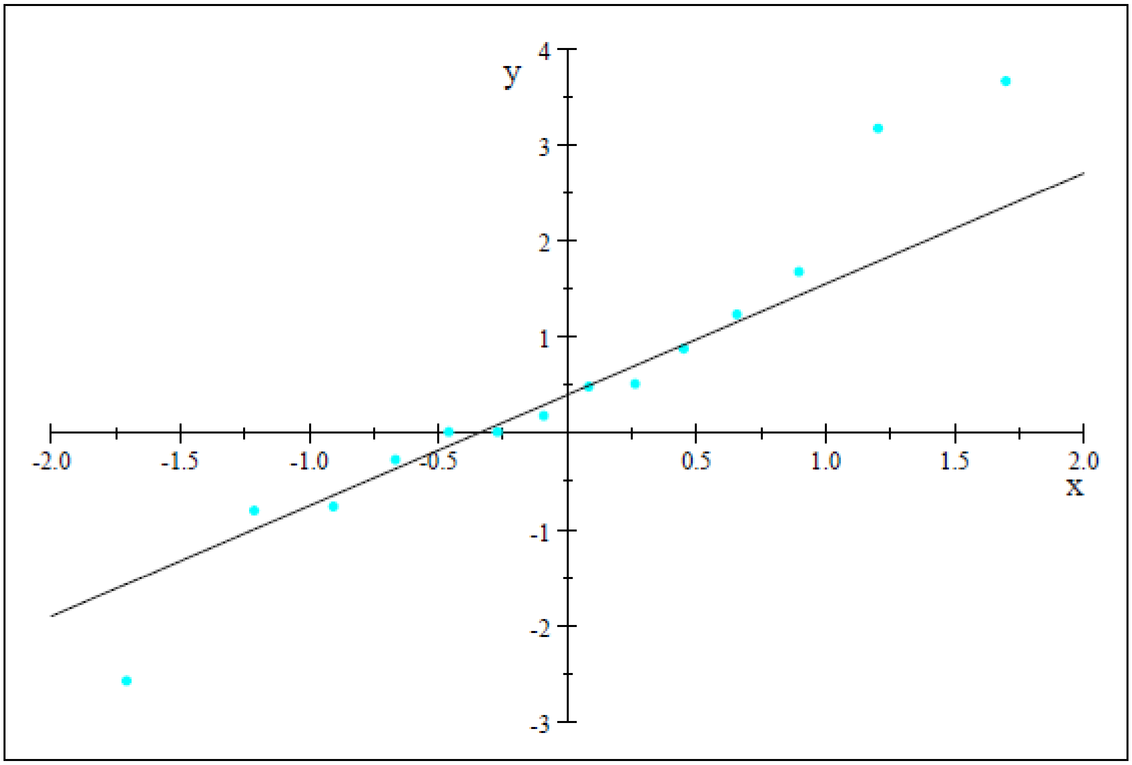
$$\left(-1.7033815541, -\frac{11\sqrt{2}}{6}\right), \ \left(1.2079022754, \sqrt{10}\right), \text{ and } \left(1.7033815541, \frac{2\sqrt{30}}{3}\right).$$

A simple fitting of a line to the eleven points, we have that

$$\widehat{\theta}_{i:(a-1)(b-1)-1} = 0.4007897323 + 1.1531953369\delta_{i:(a-1)(b-1)-1}.$$

Plotting this line with our points, we obtain the graph in Figure 2.2.

Figure 2.2: Montgomery Example, Probability Plot and Fitted Line 11 Points



The three points

$$\left(-1.7033815541, -\frac{11\sqrt{2}}{6}\right),\ \left(1.2079022754, \sqrt{10}\right), \text{ and } \left(1.7033815541, \frac{2\sqrt{30}}{3}\right).$$

are associated with the contrast estimators $(\widehat{\tau}_2^*)_3$, $(\widehat{\tau}_1^*)_2$, and $(\widehat{\tau}_1^*)_1$, respectively. This plot provides evidence that there is no interaction between the two factors but there is effects due to the two factors.

Example 2:

Kutner, Nachtsheim, Neter, and Li (2005) on page 890 state in Exercise 20.8 that "A food Technologist, testing storage capabilities for a newly developed type of imitation sausage made from soybeans, conducted an experiment to test the effects of humidity level (factor A) and temperature level (factor B) in the freezer compartment on color change in the sausage. Three humidity levels and four temperature levels were considered. Five hundred sausages were stored at each of the 12 humidity-temperature combinations for 90 days. At the end of the storage period, the researcher determined the proportion of sausages for each humidity-temperature combination that exhibited color changes. The researcher transformed the data by means of the arcsine transformation to stabilize the variances. The transformed data $Y' = 2\arcsin\sqrt{Y}$ follow."

Table 2.2: Kutner's Exercise 20.8

	Temperature level			
Humidity level	j=1	j=2	j=3	j=4
i=1	13.9	14.2	20.5	24.8
i=2	15.7	16.3	21.7	23.6
i=3	15.1	15.4	19.9	26.1

We see that

$$
\begin{aligned}
\overline{Y}_{1.} &= \frac{13.9 + 14.2 + 20.5 + 24.8}{4} = 18.350;\\
\overline{Y}_{2.} &= \frac{15.7 + 16.3 + 21.7 + 23.6}{4} = 19.325;\\
\overline{Y}_{3.} &= \frac{15.1 + 15.4 + 19.9 + 26.1}{4} = 19.125;\\
\overline{Y}_{.1} &= \frac{13.9 + 15.7 + 15.1}{3} = 14.9;\\
\overline{Y}_{.2} &= \frac{14.2 + 16.3 + 15.4}{3} = 15.3;\\
\overline{Y}_{.3} &= \frac{20.5 + 21.7 + 19.9}{3} = 20.7;\\
\overline{Y}_{.4} &= \frac{24.8 + 23.6 + 26.1}{3} = 24.8\overline{3};\\
Y_{..} &= 13.9 + 14.2 + 20.5 + 24.8 + 15.7 + 16.3\\
&\quad + 21.7 + 23.6 + 15.1 + 15.4 + 19.9 + 26.1\\
&= 227.2; \text{ and}\\
\overline{Y}_{..} &= \frac{227.2}{12} = 18.9\overline{3}
\end{aligned}
$$

Assuming interaction between the two factors has the form

$$(\tau_{12})_{ij} = \lambda\,(\tau_1)_i\,(\tau_2)_j\,,$$

then the least squares estimates of the parameters μ, $(\tau_1)_1$, $(\tau_1)_2$,$(\tau_1)_3$, $(\tau_2)_1$, $(\tau_2)_2$, $(\tau_2)_3$, and $(\tau_2)_4$ are

$$
\begin{aligned}
\widehat{\mu} &= \overline{Y}_{..} = 18.9\overline{3};\\
(\widehat{\tau}_1)_1 &= \overline{Y}_{1.} - \overline{Y}_{..} = 18.350 - 18.9\overline{3} = -0.58\overline{3};\\
(\widehat{\tau}_1)_2 &= \overline{Y}_{2.} - \overline{Y}_{..} = 19.325 - 18.9\overline{3} = 0.391\overline{6};\\
(\widehat{\tau}_1)_3 &= \overline{Y}_{3.} - \overline{Y}_{..} = 19.125 - 18.9\overline{3} = 0.191\overline{6};\\
(\widehat{\tau}_2)_1 &= \overline{Y}_{.1} - \overline{Y}_{..} = 14.9 - 18.9\overline{3} = -4.0\overline{3};\\
(\widehat{\tau}_2)_2 &= \overline{Y}_{.2} - \overline{Y}_{..} = 15.3 - 18.9\overline{3} = -3.6\overline{3};\\
(\widehat{\tau}_2)_3 &= \overline{Y}_{.3} - \overline{Y}_{..} = 20.7 - 18.9\overline{3} = 1.7\overline{6};\\
(\widehat{\tau}_2)_4 &= \overline{Y}_{.4} - \overline{Y}_{..} = 24.8\overline{3} - 18.9\overline{3} = 5.9.
\end{aligned}
$$

Recall that the formula to be used to obtain an estimate of λ is

$$
\widehat{\lambda} = \frac{\sum_{i=1}^{3}\sum_{j=1}^{4}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)\left(\overline{Y}_{.j} - \overline{Y}_{..}\right)Y_{ij}}{\sum_{i=1}^{3}\sum_{j=1}^{4}\left(\overline{Y}_{i.} - \overline{Y}_{..}\right)^2\left(\overline{Y}_{.j} - \overline{Y}_{..}\right)^2}.
$$

It follows that

$$
\begin{aligned}
&\sum_{i=1}^{3}\sum_{j=1}^{4}\left(\overline{Y}_{i.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.j}-\overline{Y}_{..}\right)Y_{ij}\\
&=\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.1}-\overline{Y}_{..}\right)Y_{11}+\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.2}-\overline{Y}_{..}\right)Y_{12}\\
&+\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.3}-\overline{Y}_{..}\right)Y_{13}+\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.4}-\overline{Y}_{..}\right)Y_{14}\\
&+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.1}-\overline{Y}_{..}\right)Y_{21}+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.2}-\overline{Y}_{..}\right)Y_{22}\\
&+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.3}-\overline{Y}_{..}\right)Y_{23}+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.4}-\overline{Y}_{..}\right)Y_{24}\\
&+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.1}-\overline{Y}_{..}\right)Y_{31}+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.2}-\overline{Y}_{..}\right)Y_{32}\\
&+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.3}-\overline{Y}_{..}\right)Y_{33}+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)\left(\overline{Y}_{.4}-\overline{Y}_{..}\right)Y_{34}\\
&=\left(-0.58\overline{3}\right)\left(-4.0\overline{3}\right)(13.9)+\left(-0.58\overline{3}\right)\left(-3.6\overline{3}\right)(14.2)\\
&+\left(-0.58\overline{3}\right)\left(1.7\overline{6}\right)(20.5)+\left(-0.58\overline{3}\right)(5.9)(24.8)\\
&+\left(0.391\overline{6}\right)\left(-4.0\overline{3}\right)(15.7)+\left(0.391\overline{6}\right)\left(-3.6\overline{3}\right)(16.3)\\
&+\left(0.391\overline{6}\right)\left(1.7\overline{6}\right)(21.7)+\left(0.391\overline{6}\right)(5.9)(23.6)\\
&+\left(0.191\overline{6}\right)\left(-4.0\overline{3}\right)(15.1)+\left(0.191\overline{6}\right)\left(-3.6\overline{3}\right)(15.4)\\
&+\left(0.191\overline{6}\right)\left(1.7\overline{6}\right)(19.9)+\left(0.191\overline{6}\right)(5.9)(26.1)\\
&=-8.27099996
\end{aligned}
$$

and

$$
\begin{aligned}
&\sum_{i=1}^{3}\sum_{j=1}^{4}\left(\overline{Y}_{i.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.j}-\overline{Y}_{..}\right)^2\\
&=\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.1}-\overline{Y}_{..}\right)^2+\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.2}-\overline{Y}_{..}\right)^2\\
&+\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.3}-\overline{Y}_{..}\right)^2+\left(\overline{Y}_{1.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.4}-\overline{Y}_{..}\right)^2\\
&+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.1}-\overline{Y}_{..}\right)^2+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.2}-\overline{Y}_{..}\right)^2\\
&+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.3}-\overline{Y}_{..}\right)^2+\left(\overline{Y}_{2.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.4}-\overline{Y}_{..}\right)^2\\
&+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.1}-\overline{Y}_{..}\right)^2+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.2}-\overline{Y}_{..}\right)^2\\
&+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.3}-\overline{Y}_{..}\right)^2+\left(\overline{Y}_{3.}-\overline{Y}_{..}\right)^2\left(\overline{Y}_{.4}-\overline{Y}_{..}\right)^2\\
&=\left(-0.58\overline{3}\right)^2\left(-4.0\overline{3}\right)^2+\left(-0.58\overline{3}\right)^2\left(-3.6\overline{3}\right)^2\\
&+\left(-0.58\overline{3}\right)^2\left(1.7\overline{6}\right)^2+\left(-0.58\overline{3}\right)^2(5.9)^2\\
&+\left(0.391\overline{6}\right)^2\left(-4.0\overline{3}\right)^2+\left(0.391\overline{6}\right)^2\left(-3.6\overline{3}\right)^2\\
&+\left(0.391\overline{6}\right)^2\left(1.7\overline{6}\right)^2+\left(0.391\overline{6}\right)^2(5.9)^2\\
&+\left(0.191\overline{6}\right)^2\left(-4.0\overline{3}\right)^2+\left(0.191\overline{6}\right)^2\left(-3.6\overline{3}\right)^2\\
&+\left(0.191\overline{6}\right)^2\left(1.7\overline{6}\right)^2+\left(0.191\overline{6}\right)^2(5.9)^2\\
&=35.7500833.
\end{aligned}
$$

Thus, we have

$$\widehat{\lambda}=\frac{-8.27099996}{35.7500833}=-0.2313561032.$$

It follows that the SST, SSA, SSB, and $SSAB^*$ are

$$
\begin{aligned}
SST &= \sum\nolimits_{i=1}^{a} \sum\nolimits_{j=1}^{b} \left(Y_{ij} - \overline{Y}_{..}\right)^2 = \left(13.9 - 18.9\overline{3}\right)^2 + \left(14.2 - 18.9\overline{3}\right)^2 \\
&+ \left(20.5 - 18.9\overline{3}\right)^2 + \left(24.8 - 18.9\overline{3}\right)^2 + \left(15.7 - 18.9\overline{3}\right)^2 \\
&+ \left(16.3 - 18.9\overline{3}\right)^2 + \left(21.7 - 18.9\overline{3}\right)^2 + \left(23.6 - 18.9\overline{3}\right)^2 \\
&+ \left(15.1 - 18.9\overline{3}\right)^2 + \left(15.4 - 18.9\overline{3}\right)^2 + \left(19.9 - 18.9\overline{3}\right)^2 \\
&+ \left(26.1 - 18.9\overline{3}\right)^2 \\
&= 210.9066667, \\
SSA &= \sum\nolimits_{i=1}^{a} \left(\overline{Y}_{i.} - \overline{Y}_{..}\right)^2 = \left(-0.58\overline{3}\right)^2 + \left(0.391\overline{6}\right)^2 + \left(0.191\overline{6}\right)^2 \\
&= 0.5304166663, \\
SSB &= \sum\nolimits_{j=1}^{b} \left(\overline{Y}_{.j} - \overline{Y}_{..}\right)^2 = \left(-4.0\overline{3}\right)^2 + \left(-3.6\overline{3}\right)^2 + \left(1.7\overline{6}\right)^2 + (5.9)^2 \\
&= 67.39999996, \text{ and} \\
SSAB^* &= \sum\nolimits_{i=1}^{a} \sum\nolimits_{j=1}^{b} \widehat{\lambda}^2 \left(\overline{Y}_{i.} - \overline{Y}_{..}\right)^2 \left(\overline{Y}_{.j} - \overline{Y}_{..}\right)^2 \\
&= (-0.2313561032)^2 \, (35.7500833) \\
&= 1.913546321.
\end{aligned}
$$

We then have

$$
\begin{aligned}
SSE^* &= SST - SSA - SSB - SSAB^* \\
&= 210.9066667 - 0.5304166663 - 67.39999996 - 1.913546321 \\
&= 141.0627038.
\end{aligned}
$$

The associated mean squares are

$$\begin{aligned} MSA &= \frac{0.5304166663}{3-1} = 0.2652083332; \\ MSB &= \frac{67.39999996}{4-1} = 22.46666665; \\ MSAB^{*} &= \frac{1.913546321}{1} = 1.913546321; \text{ and} \\ MSE^{*} &= \frac{141.0627038}{(3)(4)-3-4} = 28.21254076. \end{aligned}$$

The observed value of $F = MSAB^{*}/MSE^{*}$ is

$$F_{observed} = \frac{1.913546321}{28.21254076} = 0.06782608973.$$

We see that if $\lambda = 0$, then the probability of the random variable $F_{1,5}$ is greater than or equal to $F_{observed}$ is

$$\begin{aligned} P\left(F_{1,5} \geq F_{observed}\right) &= 1 - P\left(F_{1,5} < F_{observed}\right) \\ &= 1 - \text{FDist}\left(0.06782608973; 1, 5\right) \\ &= 0.8049139196. \end{aligned}$$

These results suggest there is no two factor interaction.

Lets assume the reduced model of no interaction between Factors A and B. Our model is

$$\mu_{ij} = \mu + (\tau_1)_i + (\tau_2)_j\,.$$

The design matrix is

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & -1 & -1 & -1 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 0 \\ 1 & -1 & -1 & 0 & 0 & 1 \\ 1 & -1 & -1 & -1 & -1 & -1 \end{bmatrix}.$$

Our least squares estimates are

$$\left(\mathbf{X^T X}\right)^{-1} \mathbf{X^T y} = \begin{bmatrix} 18.93333333 \\ -0.5833333333 \\ 0.391666\,6667 \\ -4.033\,333333 \\ -3.633333333 \\ 1.766\,666667 \end{bmatrix}.$$

Our total sum of squares, the sums of squares due to Factors A and B, and the sum of squares due to error are

$$\begin{aligned}
SST &= (12)(18.93333333) = 227.2; \\
SSA &= (-0.5833333333)^2 + (0.3916666667)^2 + (0.19166666667)^2 \\
&= 0.5304166667; \\
SSB &= (-4.033\,333333)^2 + (-3.633333333)^2 + (1.766666667)^2 + (5.9)^2 \\
&= 67.39999996; \text{ and} \\
SSE &= SST - SSA - SSB = 159.2695834.
\end{aligned}$$

We observe that

$$\begin{aligned}
\frac{SSA/(a-1)}{SSE/((a-1)(b-1))} &= \frac{0.5304166667/(3-1)}{159.2695834/((3-1)(4-1))} \\
&= 0.009990922103; \text{ and} \\
\frac{SSB/(b-1)}{SSE/((a-1)(b-1))} &= \frac{67.39999996/(4-1)}{159.2695834/((3-1)(4-1))} \\
&= 0.8463637388.
\end{aligned}$$

The associated p-values are, respectively,

$$\begin{aligned}
P(F_{2,6} \geq 0.009990922103) &= 1 - \text{FDist}(0.009990922103; 2, 6) \\
&= 0.9900752561; \text{ and} \\
P(F_{3,6} \geq 0.8463637388) &= 1 - \text{FDist}(0.8463637388; 3, 6) \\
&= 0.5168608443.
\end{aligned}$$

These results suggest that there is no effect due to either of the two factors.

For the full model, the design matrix for the full model and our data in vector form are

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & -1 & -1 & -1 & 0 & 0 & 0 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & -1 \\ 1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \text{ and } \mathbf{y} = \begin{bmatrix} 13.9 \\ 14.2 \\ 20.5 \\ 24.8 \\ 15.7 \\ 16.3 \\ 21.7 \\ 23.6 \\ 15.1 \\ 15.4 \\ 19.9 \\ 26.1 \end{bmatrix}.$$

The matrix $\mathbf{P}$ associated with $\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}$ is

$$\mathbf{P} = \begin{bmatrix} \frac{\sqrt{12}}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{18}}{18} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & 0 & -\frac{2\sqrt{18}}{18} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{18}}{18} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{18}}{36} & \frac{\sqrt{6}}{12} & \frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{1}{2} & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{18}}{36} & \frac{\sqrt{6}}{12} & 0 & -\frac{1}{3} & 0 & -\frac{\sqrt{3}}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{18}}{36} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{3}}{6} & \frac{1}{6} & -\frac{1}{2} & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{18}}{36} & -\frac{\sqrt{6}}{12} & \frac{\sqrt{3}}{6} & \frac{1}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{18}}{36} & -\frac{\sqrt{6}}{12} & 0 & -\frac{1}{3} & 0 & \frac{\sqrt{3}}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{18}}{36} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{3}}{6} & \frac{1}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} \end{bmatrix}.$$

The least squares estimates for the main effects and interaction is given by

$$\widehat{\theta} = \left(\mathbf{X^T X}\right)^{-1} \mathbf{X^T y} = \begin{bmatrix} 18.9\overline{3} \\ -0.58\overline{3} \\ 0.391\overline{6} \\ -4.0\overline{3} \\ -3.6\overline{3} \\ 1.7\overline{6} \\ -0.41\overline{6} \\ -0.51\overline{6} \\ 0.38\overline{3} \\ 0.408\overline{3} \\ 0.608\overline{3} \\ 0.608\overline{3} \end{bmatrix}$$

the contrasts of the main effects and interactions are

$$\theta^* = \mathbf{P}^{-1}\theta = \begin{bmatrix} 2\sqrt{3}\theta_1 \\ \sqrt{6}\,(\theta_2+\theta_3) \\ \sqrt{2}\,(\theta_2-\theta_3) \\ 2\,(\theta_4+\theta_5+\theta_6) \\ \frac{\sqrt{6}}{2}\,(\theta_4-\theta_6) \\ \frac{\sqrt{2}}{2}\,(\theta_4-2\theta_5+\theta_6) \\ \sqrt{2}\,(\theta_7+\theta_8+\theta_9+\theta_{10}+\theta_{11}+\theta_{12}) \\ \frac{\sqrt{6}}{3}\,(\theta_7+\theta_8+\theta_9-\theta_{10}-\theta_{11}-\theta_{12}) \\ \frac{\sqrt{3}}{2}\,(\theta_7-\theta_9+\theta_{10}-\theta_{12}) \\ \frac{1}{2}\,(\theta_7-2\theta_8+\theta_9+\theta_{10}-2\theta_{11}+\theta_{12}) \\ \frac{1}{2}\,(\theta_7-\theta_9-\theta_{10}+\theta_{12}) \\ \frac{\sqrt{3}}{6}\,(\theta_7-2\theta_8+\theta_9-\theta_{10}+2\theta_{11}-\theta_{12}) \end{bmatrix}.$$

The coordinates of the random vector $\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta}$ of estimators of the vector θ^* of the contrasts of the main effects and interactions are independent. The estimates for these contrasts are

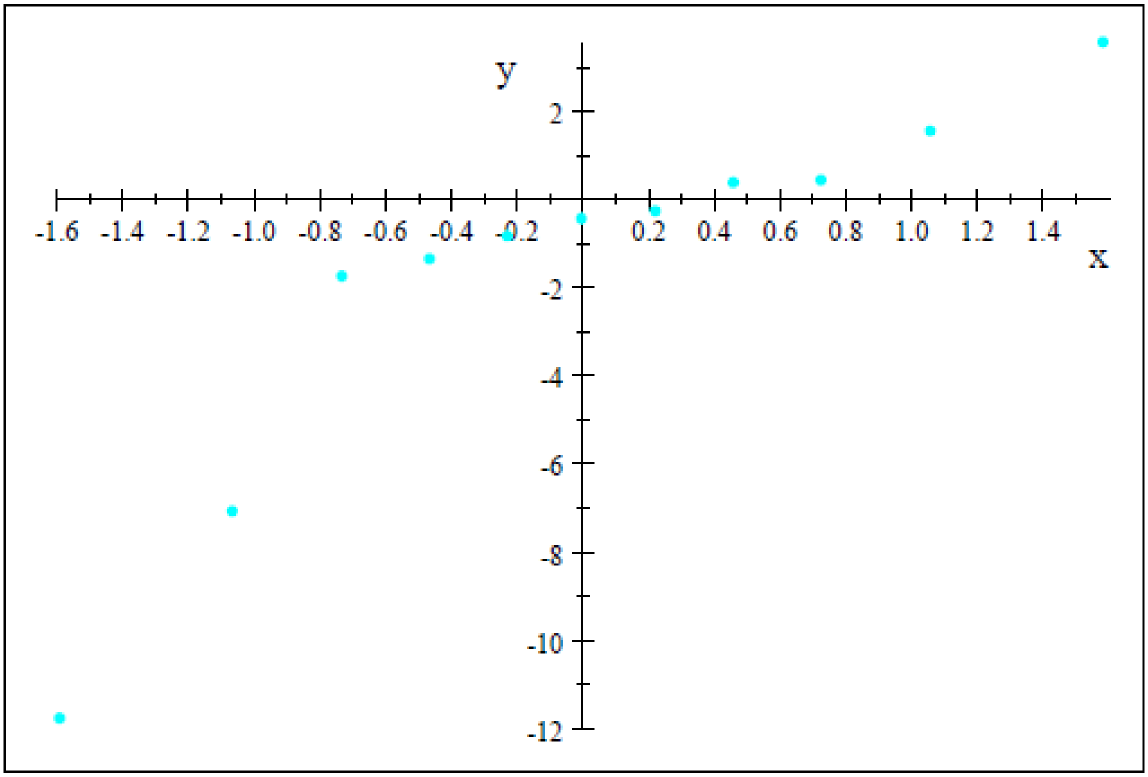
$$\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta} = \begin{bmatrix} 65.58699059 \\ -0.4694855341 \\ -1.378858223 \\ -11.8 \\ -7.103520254 \\ 3.535533906 \\ 1.520279580 \\ -1.775880064 \\ -0.8660254038 \\ 0.4 \\ -0.3 \\ 0.3464101615 \end{bmatrix}.$$

Removing the estimate $\widehat{\theta}_1^* = 65.58699059$, we have the 11×1 vector of ordered estimates of the given linear contrasts of the main effects and interactions along with the plotting positions for the corresponding normal probability plot given in the following 11×2 matrix.

$$\begin{bmatrix} -1.5864363519 & -11.8 \\ -1.0619165201 & -7.103520254 \\ -0.7288394047 & -1.775880064 \\ -0.4619783072 & -1.378858223 \\ -0.2248908792 & -0.8660254038 \\ 0 & -0.4694855341 \\ 0.2248908792 & -0.3 \\ 0.4619783072 & 0.3464101615 \\ 0.7288394047 & 0.4 \\ 1.0619165201 & 1.520279580 \\ 1.5864363519 & 3.535533906 \end{bmatrix}.$$

A plot of these points is given in the following figure.

Figure 2.3: Kutner Example, Probability Plot

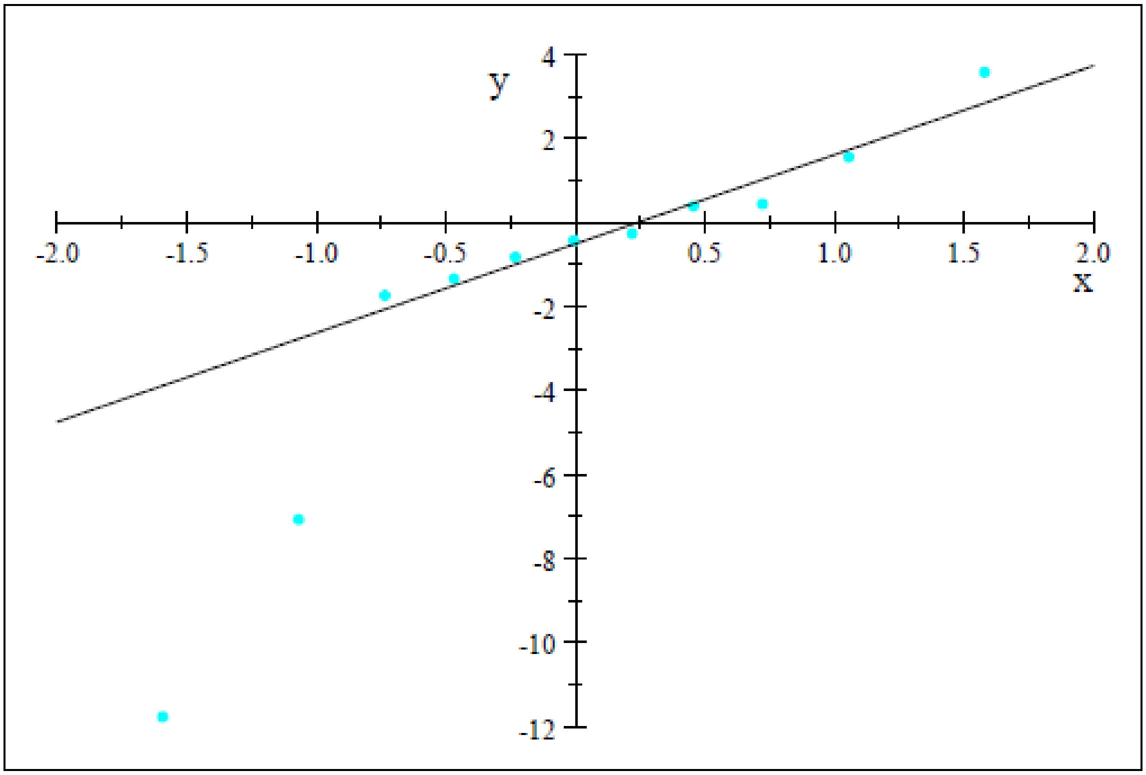


All the points seem to be plotting about a line except for the points with coordinates $(-1.5864363519, -11.8)$ and $(-1.0619165201, -7.103520254)$. Using the other nine points, we estimate the line to be

$$y = -0.5107289617 + 2.117744632x.$$

A plot of this line along with our normal probability plot of the data is shown in the following figure.

Figure 2.4: Kutner Example, Probability Plot and Fitted Line 9 Points

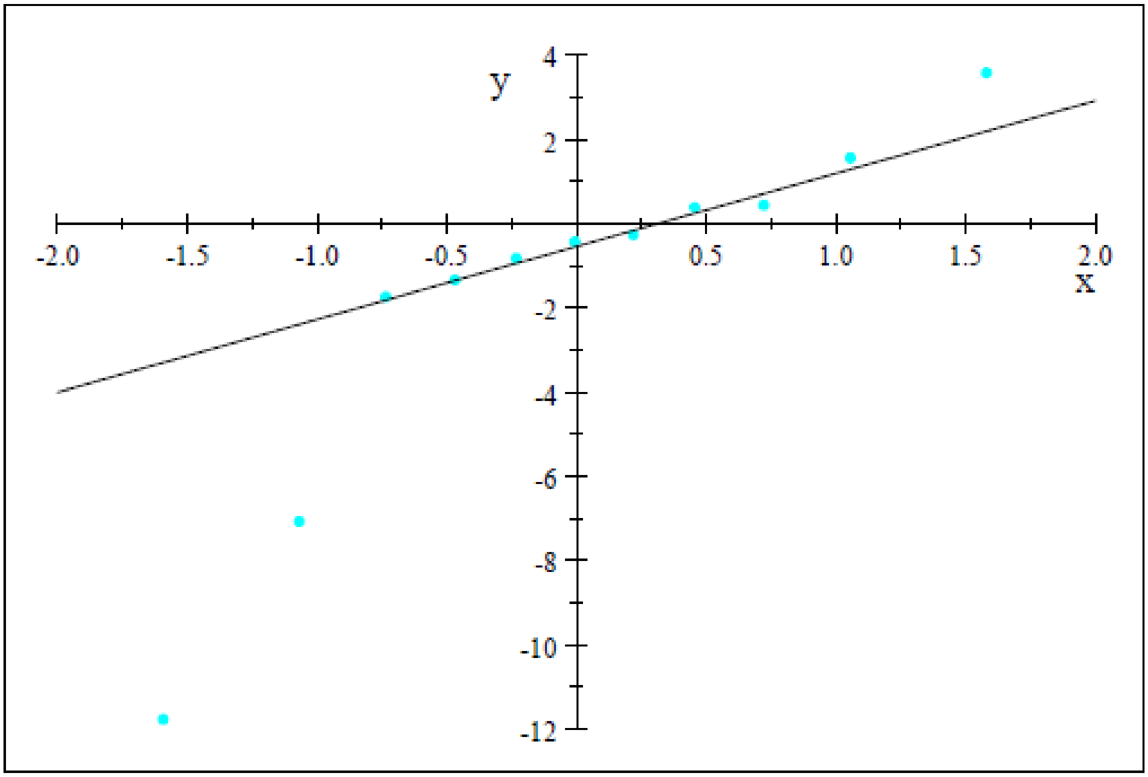


The point with coordinates $(1.5864363519, 3.535533906)$ may also be an outlier. To examine this possibility, we used the other eight points to estimate the line. This line is

$$y = -0.5451442881 + 1.730451299x.$$

A plot of this line along with the normal probability plot of the data is given in the following figure.

Figure 2.5: Kutner Example, Probability Plot and Fitted Line 8 Points



The contrast associated with the three estimates

$$\widehat{\theta}_4^*,\ \widehat{\theta}_5^*,\ \text{and}\ \widehat{\theta}_6^*$$

are, respectively,

$$2\left(\theta_4+\theta_5+\theta_6\right),\ \frac{\sqrt{6}}{2}\left(\theta_4-\theta_6\right),\ \text{and}\ \frac{\sqrt{2}}{2}\left(\theta_4-2\theta_5+\theta_6\right).$$

These contrast are all associated with Factor B: temperature. The plot shows no evidence there is an effect due to Factor A (pressure) or interactions between Factors A and B which is expected.

2.7 Conclusion

A method for analyzing unreplicated two factor experiments using selected contrasts has been presented. This method is based on a normal probability plot of the estimates the main effect contrasts and the interaction contrasts. This method provides the researcher a method of identifying the contrasts that are significantly different from zero. As was illustrated, each contrast is a contrast of a particular main effect or interaction. Hence, if a contrast is identified as being significantly different from zero, then it follows that the associated main effect or interaction is different from zero.

CHAPTER 3

THREE FACTOR EXPERIMENTS

3.1 Introduction

The model for a three factor experiment ($k = 3$) under the additive model expresses the response variable Y_{ijrs} as

$$Y_{ijrs} = \mu_{ijr} + \epsilon_{ijrs}$$

with

$$\mu_{ijr} = \mu + (\tau_1)_i + (\tau_2)_j + (\tau_3)_r + (\tau_{12})_{ij} + (\tau_{13})_{ir} + (\tau_{23})_{jr} + (\tau_{123})_{ijr}$$

and ϵ_{ijrs} iid $N(0, \sigma^2)$ for $i = 1, \ldots, a$, $j = 1, \ldots, b$, $r = 1, \ldots, c$, and $s = 1, \ldots, n$. It is assumed that main effects and interactions are such that

$$\begin{gathered}
\sum\nolimits_{i=1}^{a} (\tau_1)_i = 0;\ \sum\nolimits_{j=1}^{b} (\tau_2)_j = 0;\ \sum\nolimits_{r=1}^{c} (\tau_3)_r = 0; \\
\sum\nolimits_{j=1}^{b} (\tau_{12})_{ij} = 0 \text{ for } i = 1, \ldots, a;\ \sum\nolimits_{i=1}^{a} (\tau_{12})_{ij} = 0 \text{ for } j = 1, \ldots, b; \\
\sum\nolimits_{r=1}^{c} (\tau_{13})_{ir} = 0 \text{ for } i = 1, \ldots, a;\ \sum\nolimits_{i=1}^{a} (\tau_{13})_{ir} = 0 \text{ for } r = 1, \ldots, c; \\
\sum\nolimits_{r=1}^{c} (\tau_{23})_{jr} = 0 \text{ for } j = 1, \ldots, b;\ \sum\nolimits_{j=1}^{b} (\tau_{23})_{jr} = 0 \text{ for } r = 1, \ldots, c; \\
\sum\nolimits_{r=1}^{c} (\tau_{123})_{ijr} = 0 \text{ for } i = 1, \ldots, a,\ j = 1, \ldots, b; \\
\sum\nolimits_{j=1}^{b} (\tau_{123})_{ijr} = 0 \text{ for } i = 1, \ldots, a,\ r = 1, \ldots, c; \text{ and} \\
\sum\nolimits_{i=1}^{a} (\tau_{123})_{ijr} = 0 \text{ for } j = 1, \ldots, b,\ r = 1, \ldots, c.
\end{gathered}$$

This is referred to as the full model. One can reduce the model by assuming some of the interactions are zero. If this is done, we will refer to this model as the reduced model. We also assume that the ϵ_{ijrs}'s are independent and $\epsilon_{ijrs} \sim N(0, \sigma^2)$. We refer to these assumptions as the independent normal model. The design is an unreplicated one if $n = 1$. Using matrix notation, we can write our additive model in the form

$$\mathbf{Y} = \mathbf{X}\theta + \epsilon,$$

where $\mathbf{Y}$ is the $abcn \times 1$ vector of observations, $\mathbf{X}$ is the $abcn \times abc$ design matrix, θ is the $abc \times 1$ vector of model parameters, and ϵ is the $abcn \times 1$ vector of error terms. We are interested in studying the case in which $n = 1$.

A study in which there is only one replicate per treatment does not allow one to perform an analysis of variance if the full model is assumed. For these data, there is not enough informations in the data to independently estimate the main effects and interactions and the common variance. Two methods have been suggested in the literature for analyzing the data from a design without replicates. The first of these is an extention of Tukey's method used to test for non-additivity. This is discussed in the next section. The second of these analyzes the data under a reduced model. This will be examined in Section 3. We present a third method in Section 4. In Section 5, we discuss the analysis of 3^k factorial designs. Some examples are given in Section 6.

3.2 Tukey's Method for Three Factors

Tukey (1949) method can be extended to develop tests for non-additivity for three factor experiments. In this case, one is to assume that the two and three factor interactions can be expressed in terms of the main effects and the parameters λ_{12}, λ_{13}, λ_{23}, and λ_{123}. Under Tukey's model, it is assumed that

$$\begin{aligned}
(\tau_{12})_{ij} &= \lambda_{12}\,(\tau_1)_i\,(\tau_2)_j\,;\ \ (\tau_{13})_{ir} = \lambda_{13}\,(\tau_1)_i\,(\tau_3)_r\,; \\
(\tau_{23})_{jr} &= \lambda_{23}\,(\tau_2)_j\,(\tau_3)_r\,; \text{ and } \ (\tau_{123})_{ijr} = \lambda_{123}\,(\tau_1)_i\,(\tau_2)_j\,(\tau_3)_r\,.
\end{aligned}$$

In this model, there are $a+b+c+5$ parameters including the common variance to be estimated. To determine these estimates using least squares, we define the function

$$
\begin{aligned}
Q &= Q\left(\mu, (\tau_1)_1, \ldots, (\tau_1)_a, (\tau_2)_1, \ldots, (\tau_2)_b, (\tau_3)_1, \ldots, (\tau_3)_c, \lambda_{12}, \lambda_{13}, \lambda_{23}, \lambda_{123}\right) \\
&= \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{r=1}^{c} (Y_{ij} - \mu - (\tau_1)_i - (\tau_2)_j - (\tau_3)_r - \lambda_{12} (\tau_1)_i (\tau_2)_j \\
&\quad - \lambda_{13} (\tau_1)_i (\tau_3)_r - \lambda_{23} (\tau_2)_j (\tau_3)_r - \lambda_{123} (\tau_1)_i (\tau_2)_j (\tau_3)_r)^2
\end{aligned}
$$

The least square estimates are the solutions to the following system of equations.

$$
\begin{aligned}
\frac{\partial Q}{\partial \mu} &= 0;\ \frac{\partial Q}{\partial (\tau_1)_i} = 0;\ \frac{\partial Q}{\partial (\tau_2)_j} = 0;\ \frac{\partial Q}{\partial (\tau_3)_j} = 0; \\
\frac{\partial Q}{\partial \lambda_{12}} &= 0;\ \frac{\partial Q}{\partial \lambda_{13}} = 0;\ \frac{\partial Q}{\partial \lambda_{23}} = 0;\text{ and } \frac{\partial Q}{\partial \lambda_{123}} = 0.
\end{aligned}
$$

It follows that the estimators for the model parameters $(\tau_1)_i$, $(\tau_2)_j$, $(\tau_3)_r$, λ_{12}, λ_{13}, λ_{23}, and λ_{123} are

$$
\begin{aligned}
(\widehat{\tau}_1)_i &= \overline{Y}_{i..} - \overline{Y}_{...}; \\
(\widehat{\tau}_2)_j &= \overline{Y}_{.j.} - \overline{Y}_{...}; \\
(\widehat{\tau}_3)_r &= \overline{Y}_{..r} - \overline{Y}_{...}; \\
\widehat{\lambda}_{12} &= \frac{\sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{r=1}^{c} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right) \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) Y_{ijr}}{c \sum_{i=1}^{a} \sum_{j=1}^{b} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2 \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2}; \\
\widehat{\lambda}_{13} &= \frac{\sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{r=1}^{c} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right) \left(\overline{Y}_{..r} - \overline{Y}_{...}\right) Y_{ijr}}{b \sum_{i=1}^{a} \sum_{r=1}^{c} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2 \left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2}; \\
\widehat{\lambda}_{23} &= \frac{\sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{r=1}^{c} \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) \left(\overline{Y}_{..r} - \overline{Y}_{...}\right) Y_{ijr}}{a \sum_{j=1}^{b} \sum_{r=1}^{c} \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2 \left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2};\text{ and} \\
\widehat{\lambda}_{123} &= \frac{\sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{r=1}^{c} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right) \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) \left(\overline{Y}_{..r} - \overline{Y}_{...}\right) Y_{ijr}}{\sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{r=1}^{c} \left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2 \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2 \left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2}.
\end{aligned}
$$

We can now express Y_{ijr} as

$$\begin{aligned}
Y_{ijr} &= \overline{Y}_{...} + \left(\overline{Y}_{i..} - \overline{Y}_{...}\right) + \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) + \left(\overline{Y}_{..r} - \overline{Y}_{...}\right) \\
&\quad + \widehat{\lambda}_{12}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) + \widehat{\lambda}_{13}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right) \\
&\quad + \widehat{\lambda}_{23}\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right) + \widehat{\lambda}_{123}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right) + \widehat{\epsilon}_{ijr}.
\end{aligned}$$

It follows that $\widehat{\epsilon}_{ijr}$ can be expressed as

$$\begin{aligned}
\widehat{\epsilon}_{ijr} &= Y_{ijr} - \overline{Y}_{...} - \left(\overline{Y}_{i..} - \overline{Y}_{...}\right) - \left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) - \left(\overline{Y}_{..r} - \overline{Y}_{...}\right) \\
&\quad - \widehat{\lambda}_{12}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right) - \widehat{\lambda}_{13}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right) \\
&\quad - \widehat{\lambda}_{23}\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right) - \widehat{\lambda}_{123}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)
\end{aligned}$$

The total sum of squares SST can be partitioned into the follow sums of squares.

$$\begin{aligned}
SSA &= bc\sum\nolimits_{i=1}^{a}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2 \text{ with } df_{SSA} = a-1; \\
SSB &= ac\sum\nolimits_{j=1}^{b}\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2 \text{ with } df_{SSB} = b-1; \\
SSC &= ab\sum\nolimits_{r=1}^{c}\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2 \text{ with } df_{SSC} = c-1; \\
SSAB^* &= c\sum\nolimits_{i=1}^{a}\sum\nolimits_{j=1}^{b}\widehat{\lambda}_{12}^2\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2 \\
SSAC^* &= b\sum\nolimits_{i=1}^{a}\sum\nolimits_{r=1}^{c}\widehat{\lambda}_{13}^2\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2 \\
SSBC^* &= a\sum\nolimits_{j=1}^{b}\sum\nolimits_{r=1}^{c}\widehat{\lambda}_{23}^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2; \\
SSABC^* &= \sum\nolimits_{i=1}^{a}\sum\nolimits_{j=1}^{b}\sum\nolimits_{r=1}^{c}\widehat{\lambda}_{123}^2\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2; \\
&\quad \text{and} \\
SSE^* &= SST - SSA - SSB - SSC - SSAB^* - SSAC^* - SSBC^* - SSABC^*,
\end{aligned}$$

where

$$\begin{aligned}
df_{SSAB^*} &= df_{SSAC^*} = df_{SSBC^*} = df_{SSABC^*} = 1, \\
df_{SSE} &= abc - a - b - c - 2, \text{ and} \\
SST &= \sum\nolimits_{i=1}^{a}\sum\nolimits_{j=1}^{b}\sum\nolimits_{r=1}^{c}\left(Y_{ijr} - \overline{Y}_{...}\right)^2.
\end{aligned}$$

Following the derivations in Tukey (1949), one can shown that

$$\frac{SSAB^*}{\sigma^2} \sim \chi_1^2 \, , \frac{SSAC^*}{\sigma^2} \sim \chi_1^2, \frac{SSBC^*}{\sigma^2} \sim \chi_1^2, \frac{SSABC^*}{\sigma^2} \sim \chi_1^2, \text{and } \frac{SSE^*}{\sigma^2} \sim \chi^2_{ab-a-b-c-2}.$$

The observed values of the significance levels (SLs)

$$\begin{aligned}
SL_{123} &= P\left(F_{1,abc-a-b-c-2} \geq \frac{SSABC^*/1}{SSE^*/\left(abc-a-b-c-2\right)}\right); \\
SL_{12} &= P\left(F_{1,abc-a-b-c-2} \geq \frac{SSAB^*/1}{SSE^*/\left(abc-a-b-c-2\right)}\right); \\
SL_{13} &= P\left(F_{1,abc-a-b-c-2} \geq \frac{SSAC^*/1}{SSE^*/\left(abc-a-b-c-2\right)}\right); \text{ and} \\
SL_{23} &= P\left(F_{1,abc-a-b-c-2} \geq \frac{SSBC^*/1}{SSE^*/\left(abc-a-b-c-2\right)}\right).
\end{aligned}$$

are then examined. The observed significance levels (OSLs) OSL_{123}, OSL_{12}, OSL_{13}, and OSL_{23} can be used to judge if there is strong enough evidence in the data against the null hypotheses $H_0 : \lambda_{123} = 0$, $H_0 : \lambda_{12} = 0$, $H_0 : \lambda_{13} = 0$, and $H_0 : \lambda_{23} = 0$, respectively. Note that an observed significance level is commonly referred to as a p-value.

The test for non-additivity has null and alternative hypotheses given by

$$H_0 : \lambda_{12} = \lambda_{13} = \lambda_{23} = \lambda_{123} \text{ and } H_1 :\sim H_0.$$

The statistical test has decision rule that rejects the null hypotheis in favor of the alternative hypothesis if the observed value of

$$\frac{MSAB^*}{MSE^*} \geq c_{AB} \vee \frac{MSAC^*}{MSE^*} \geq c_{AC} \vee \frac{MSBC^*}{MSE^*} \geq c_{BC} \vee \frac{MSABC^*}{MSE^*} \geq c_{ABC},$$

where

$$\begin{aligned}
MSAB^* &= \frac{SSAB^*}{1}, \; MSAC^* = \frac{SSAC^*}{1}, \; MSBC^* = \frac{SSBC^*}{1}, \\
MSABC^* &= \frac{SSABC^*}{1}, \text{ and } MSE^* = \frac{SSE^*}{ab-a-b-c-2}.
\end{aligned}$$

The size of the test α is

$$\begin{aligned}\alpha &= P\left(\frac{MSAB^*}{MSE^*} \geq c_{AB}\right) + P\left(\frac{MSAC^*}{MSE^*} \geq c_{AC}\right) \\ &\quad + P\left(\frac{MSBC^*}{MSE^*} \geq c_{BC}\right) + P\left(\frac{MSABC^*}{MSE^*} \geq c_{ABC}\right).\end{aligned}$$

If each of the critical values are selected to be the $100\,(1-\gamma)$th percentile of the appropriate F-distribution, then

$$\alpha = 4\gamma \text{ or } \gamma = \alpha/4.$$

3.3 Analyzing a Reduced Model

For the case in which $n = 1$, a reduced model can be entertained by assuming some of the parameters in the model associated with interactions are zero. Under this new assumption there is information in the data that can be used to estimate the common variance. For example, if there are no three factor interactions, our reduced model becomes

$$\mu_{ijr} = \mu + (\tau_1)_i + (\tau_2)_j + (\tau_3)_r + (\tau_{12})_{ij} + (\tau_{13})_{ir} + (\tau_{23})_{jr}\,.$$

It follows that SSE under this reduced model is the $SSABC$ under the full model. The SST can be partitioned as

$$SST = SSA + SSB + SSC + SSAB + SSAC + SSBC + SSE.$$

An ANOVA can then be used to analyze the data. There are many other possible reduced models that assumes various parameters representing interactions are zero. For example, suppose that $a = 5$ and $b = 7$.

3.4 Analysis of Contrasts

The analysis of contrast is the same for any factorial experiment. The matrix $\mathbf{P}$ is determined such that

$$\left(\mathbf{X^T X}\right)^{-1} = \mathbf{PP^T}.$$

The estimates $\widehat{\theta}$ of the vector of parameters θ for the full model are transformed into the vector of contrast

$$\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta}.$$

Under the independent normal model,

$$\widehat{\theta}^* \sim N_{abc}\left(\theta^* = \mathbf{P}^{-1}\theta, \mathbf{I}\sigma^2\right).$$

We observe that the contrasts of the estimates in the vector $\widehat{\theta}$ associated with a main effect or an interaction are the corresponding components of $\widehat{\theta}^*$. Removing the contrast associate with the overall mean in $\widehat{\theta}^*$, a normal probability plot of the remaining components can be examined. Points on the plot that provide evidence against the hypothesis $\theta^* = \mathbf{0}$ are analyzed. These points suggest that the given parameter contrast differs from zero.

3.5 Unreplicated 3^k Factorial Designs

In the analysis of a 3^k factorial experiment using contrasts, one needs the design matrix $\mathbf{X}$ to estimate the parameters in the full model and the matrix $\mathbf{P}^{-1}$ such that

$$\left(\mathbf{X^T X}\right)^{-1} = \mathbf{PP^T}.$$

However, one may have software that can be used to determine the estimates $\widehat{\theta}$ and then one can find $\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta}$. In what follows, we demonstrate that the matrix $\mathbf{P}^{-1}$ has a general form.

Define the sequence of matrices, $\mathbf{B}_{2^0}, \mathbf{B}_{2^1}, \ldots, \mathbf{B}_{2^k}$ as

$$
\begin{aligned}
\mathbf{B}_{2^0} &= \frac{1}{3^k}[1], \\
\mathbf{B}_{2^1} &= \frac{1}{3^k}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} = \begin{bmatrix} 2\mathbf{B}_{2^0} & -\mathbf{B}_{2^0} \\ -\mathbf{B}_{2^0} & 2\mathbf{B}_{2^0} \end{bmatrix}, \\
\mathbf{B}_{2^2} &= \frac{1}{3^k}\begin{bmatrix} 4 & -2 & -2 & 1 \\ -2 & 4 & 1 & -2 \\ -2 & 1 & 4 & -2 \\ 1 & -2 & -2 & 4 \end{bmatrix} = \begin{bmatrix} 2\mathbf{B}_{2^1} & -\mathbf{B}_{2^1} \\ -\mathbf{B}_{2^1} & 2\mathbf{B}_{2^1} \end{bmatrix}, \\
\mathbf{B}_{2^3} &= \frac{1}{3^k}\begin{bmatrix} 8 & -4 & -4 & 2 & -4 & 2 & 2 & -1 \\ -4 & 8 & 2 & -4 & 2 & -4 & -1 & 2 \\ -4 & 2 & 8 & -4 & 2 & -1 & -4 & 2 \\ 2 & -4 & -4 & 8 & -1 & 2 & 2 & -4 \\ -4 & 2 & 2 & -1 & 8 & -4 & -4 & 2 \\ 2 & -4 & -1 & 2 & -4 & 8 & 2 & -4 \\ 2 & -1 & -4 & 2 & -4 & 2 & 8 & -4 \\ -1 & 2 & 2 & -4 & 2 & -4 & -4 & 8 \end{bmatrix} = \begin{bmatrix} 2\mathbf{B}_{2^2} & -\mathbf{B}_{2^2} \\ -\mathbf{B}_{2^2} & 2\mathbf{B}_{2^2} \end{bmatrix}, \\
&\vdots \\
\mathbf{B}_{2^k} &= \begin{bmatrix} 2\mathbf{B}_{2^{k-1}} & -\mathbf{B}_{2^{k-1}} \\ -\mathbf{B}_{2^{k-1}} & 2\mathbf{B}_{2^{k-1}} \end{bmatrix}.
\end{aligned}
$$

The matrix $\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}$ can be expressed as block diagonal matrix with 2^k matrices on the block diagonal. The first block matrix is $\mathbf{B}_{2^0}$, the matrix $\mathbf{B}_{2^1}$ is the next $\binom{k}{1}$ block matrices, the matrix $\mathbf{B}_{2^2}$ is the next $\binom{k}{2}$ block matrices etc. It follows that $\mathbf{P}$ is a block diagonal matrix of the same construct as $\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}$ with $\mathbf{B}_{2^i}$ replaced with $\mathbf{P}_{2^i}$ for $i = 1, \ldots, k$, where

$$\mathbf{B}_{2^i} = \mathbf{P}_{2^i}\mathbf{P}_{2^i}^{\mathbf{T}}.$$

for $i = 0, 1, 2, \ldots, k$.

3.6 Example

Montgomery (1997) gives an example of a three factor experiment in which $n = 1$. He states in his example 6-3 that "the process engineer can control three variables during the filling process: the percent carbonation(A), the operating pressure in the filler (B), and the bottles produced per minute or the line speed (C)." His data is presented in the following table.

Table 3.1: Montgomery's Example 6-3

Operating pressure	25psi		30psi	
	Line speed		Line speed	
Percent carbonation	200	250	200	250
10	-4	-1	-1	2
12	1	3	5	11
14	9	13	16	21

We see that

$$\overline{Y}_{1..} = \frac{-4-1-1+2}{4} = -1;$$
$$\overline{Y}_{2..} = \frac{1+3+5+11}{4} = 5;$$
$$\overline{Y}_{3..} = \frac{9+13+16+21}{4} = 14.75;$$
$$\overline{Y}_{.1.} = \frac{-4+1+9-1+5+16}{6} = 4.\overline{3};$$
$$\overline{Y}_{.2.} = \frac{-1+3+13+2+11+21}{6} = 8.1\overline{6};$$
$$\overline{Y}_{..1} = \frac{-4+1+9-1+3+13}{6} = 3.5;$$
$$\overline{Y}_{..2} = \frac{-1+5+16+2+11+21}{6} = 9;$$
$$Y_{...} = -4+1+9-1+5+16-1+3+13+2+11+21$$
$$= 75; \text{ and}$$
$$\overline{Y}_{...} = \frac{75}{12} = 6.25.$$

Assuming interaction between the three factors has the form

$$\begin{aligned}
(\tau_{12})_{ij} &= \lambda_{12}\,(\tau_1)_i\,(\tau_2)_j\,, \\
(\tau_{13})_{ij} &= \lambda_{13}\,(\tau_1)_i\,(\tau_3)_r\,, \\
(\tau_{23})_{ij} &= \lambda_{23}\,(\tau_2)_j\,(\tau_3)_r\,, \text{ and} \\
(\tau_{123})_{ijr} &= \lambda_{123}\,(\tau_1)_i\,(\tau_2)_j\,(\tau_3)_r
\end{aligned}$$

then the least squares estimates of the parameters μ, $(\tau_1)_1$, $(\tau_1)_2$, $(\tau_1)_3$, $(\tau_2)_1$, $(\tau_2)_2$,

$(\tau_3)_1$, and $(\tau_3)_2$ are

$$\begin{aligned}
\widehat{\mu} &= \overline{Y}_{...} = 6.25, \\
(\widehat{\tau}_1)_1 &= \overline{Y}_{1..} - \overline{Y}_{...} = -1 - 6.25 = -7.25, \\
(\widehat{\tau}_1)_2 &= \overline{Y}_{2..} - \overline{Y}_{...} = 5 - 6.25 = -1.25, \\
(\widehat{\tau}_1)_3 &= \overline{Y}_{3..} - \overline{Y}_{...} = 14.75 - 6.25 = 8.5, \\
(\widehat{\tau}_2)_1 &= \overline{Y}_{.1.} - \overline{Y}_{...} = 4.\overline{3} - 6.25 = -1.91\overline{6}, \\
(\widehat{\tau}_2)_2 &= \overline{Y}_{.2.} - \overline{Y}_{...} = 8.1\overline{6} - 6.25 = 1.91\overline{6}, \\
(\tau_3)_1 &= \overline{Y}_{..1} - \overline{Y}_{...} = 3.5 - 6.25 = -2.75, \text{ and} \\
(\tau_3)_2 &= \overline{Y}_{..2} - \overline{Y}_{...} = 9 - 6.25 = 2.75.
\end{aligned}$$

Recall that the formula to be used to obtain an estimate of λ is

$$\begin{aligned}
\widehat{\lambda}_{12} &= \frac{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{r=1}^{c}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)Y_{ijr}}{c\sum_{i=1}^{a}\sum_{j=1}^{b}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2}, \\
\widehat{\lambda}_{13} &= \frac{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{r=1}^{c}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)Y_{ijr}}{b\sum_{i=1}^{a}\sum_{r=1}^{c}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2}, \\
\widehat{\lambda}_{23} &= \frac{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{r=1}^{c}\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)Y_{ijr}}{a\sum_{j=1}^{b}\sum_{r=1}^{c}\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2}, \text{ and} \\
\widehat{\lambda}_{123} &= \frac{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{r=1}^{c}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)Y_{ijr}}{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{r=1}^{c}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2}.
\end{aligned}$$

It follows that

$$\sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)Y_{ijr}$$

$$= 2\sum_{i=1}^{3}\sum_{j=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)Y_{ijr}$$

$$= 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)Y_{111} + 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)Y_{112}$$

$$+ 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)Y_{121} + 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)Y_{122}$$

$$+ 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)Y_{211} + 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)Y_{212}$$

$$+ 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)Y_{221} + 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)Y_{222}$$

$$+ 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)Y_{311} + 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)Y_{312}$$

$$+ 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)Y_{321} + 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)Y_{322}$$

$$= 2(-7.25)\left(-1.91\overline{6}\right)(-4) + 2(-7.25)\left(-1.91\overline{6}\right)(-1)$$

$$+ 2(-7.25)\left(1.91\overline{6}\right)(-1) + 2(-7.25)\left(1.91\overline{6}\right)(2)$$

$$+ 2(-1.25)\left(-1.91\overline{6}\right)(1) + 2(-1.25)\left(-1.91\overline{6}\right)(5)$$

$$+ 2(-1.25)\left(1.91\overline{6}\right)(3) + 2(-1.25)\left(1.91\overline{6}\right)(11)$$

$$+ 2(8.5)\left(-1.91\overline{6}\right)(9) + 2(8.5)\left(-1.91\overline{6}\right)(16)$$

$$+ 2(8.5)\left(1.91\overline{6}\right)(13) + 2(8.5)\left(1.91\overline{6}\right)(21)$$

$$= 88.16666676,$$

$$\sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)Y_{ijr}$$

$$= 2\sum_{i=1}^{3}\sum_{r=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)Y_{ijr}$$

$$= 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{111} + 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{112}$$

$$+ 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{121} + 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{122}$$

$$+ 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{211} + 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{212}$$

$$+ 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{221} + 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{222}$$

$$+ 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{311} + 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{312}$$

$$+ 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{321} + 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{322}$$

$$= 2\,(-7.25)\,(-2.75)\,(-4) + 2\,(-7.25)\,(2.75)\,(-1)$$

$$+ 2\,(-7.25)\,(-2.75)\,(-1) + 2\,(-7.25)\,(2.75)\,(2)$$

$$+ 2\,(-1.25)\,(-2.75)\,(1) + 2\,(-1.25)\,(2.75)\,(5)$$

$$+ 2\,(-1.25)\,(-2.75)\,(3) + 2\,(-1.25)\,(2.75)\,(11)$$

$$+ 2\,(8.5)\,(-2.75)\,(9) + 2\,(8.5)\,(2.75)\,(16)$$

$$+ 2\,(8.5)\,(-2.75)\,(13) + 2\,(8.5)\,(2.75)\,(21)$$

$$= 379.5,$$

$$\sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)Y_{ijr}$$

$$= 3\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)Y_{ijr}$$

$$= 3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{111}+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{112}$$

$$+ 3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{121}+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{122}$$

$$+ 3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{211}+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{212}$$

$$+ 3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{221}+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{222}$$

$$+ 3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{311}+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{312}$$

$$+ 3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{321}+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{322}$$

$$= 3\left(-1.91\overline{6}\right)(-2.75)(-4)+3\left(-1.91\overline{6}\right)(2.75)(-1)$$

$$+ 3\left(1.91\overline{6}\right)(-2.75)(-1)+3\left(1.91\overline{6}\right)(2.75)(2)$$

$$+ 3\left(-1.91\overline{6}\right)(-2.75)(1)+3\left(-1.91\overline{6}\right)(2.75)(5)$$

$$+ 3\left(1.91\overline{6}\right)(-2.75)(3)+3\left(1.91\overline{6}\right)(2.75)(11)$$

$$+ 3\left(-1.91\overline{6}\right)(-2.75)(9)+3\left(-1.91\overline{6}\right)(2.75)(16)$$

$$+ 3\left(1.91\overline{6}\right)(-2.75)(13)+3\left(1.91\overline{6}\right)(2.75)(21)$$

$$= 79.06249999,$$

$$\sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)Y_{ijr}$$
$$=\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{111}+\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{112}$$
$$+\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{121}+\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{122}$$
$$+\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{211}+\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{212}$$
$$+\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{221}+\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{222}$$
$$+\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{311}+\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{312}$$
$$+\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)Y_{321}+\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)Y_{322}$$
$$=(-7.25)\left(-1.91\overline{6}\right)(-2.75)(-4)+(-7.25)\left(-1.91\overline{6}\right)(2.75)(-1)$$
$$+(-7.25)\left(1.91\overline{6}\right)(-2.75)(-1)+(-7.25)\left(1.91\overline{6}\right)(2.75)(2)$$
$$+(-1.25)\left(-1.91\overline{6}\right)(-2.75)(1)+(-1.25)\left(-1.91\overline{6}\right)(2.75)(5)$$
$$+(-1.25)\left(1.91\overline{6}\right)(-2.75)(3)+(-1.25)\left(1.91\overline{6}\right)(2.75)(11)$$
$$+(8.5)\left(-1.91\overline{6}\right)(-2.75)(9)+(8.5)\left(-1.91\overline{6}\right)(2.75)(16)$$
$$+(8.5)\left(1.91\overline{6}\right)(-2.75)(13)+(8.5)\left(1.91\overline{6}\right)(2.75)(21)$$
$$=18.44791667,$$

$$
\begin{aligned}
&2\sum_{i=1}^{3}\sum_{j=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)^2\\
&=2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2+2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\\
&+2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2+2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\\
&+2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2+2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\\
&+2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2+2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\\
&+2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2+2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\\
&+2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2+2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\\
&=2\left(-7.25\right)^2\left(-1.91\overline{6}\right)^2+2\left(-7.25\right)^2\left(-1.91\overline{6}\right)^2\\
&+2\left(-7.25\right)^2\left(1.91\overline{6}\right)^2+2\left(-7.25\right)^2\left(1.91\overline{6}\right)^2\\
&+2\left(-1.25\right)^2\left(-1.91\overline{6}\right)^2+2\left(-1.25\right)^2\left(-1.91\overline{6}\right)^2\\
&+2\left(-1.25\right)^2\left(1.91\overline{6}\right)^2+2\left(-1.25\right)^2\left(1.91\overline{6}\right)^2\\
&+2\left(8.5\right)^2\left(-1.91\overline{6}\right)^2+2\left(8.5\right)^2\left(-1.91\overline{6}\right)^2\\
&+2\left(8.5\right)^2\left(1.91\overline{6}\right)^2+2\left(8.5\right)^2\left(1.91\overline{6}\right)^2\\
&=3714.020834,
\end{aligned}
$$

$$
\begin{aligned}
&2\sum_{i=1}^{3}\sum_{r=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)^2 \\
&= 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2 + 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2 \\
&+ 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2 + 2\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2 \\
&+ 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2 + 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2 \\
&+ 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2 + 2\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2 \\
&+ 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2 + 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2 \\
&+ 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2 + 2\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2 \\
&= 2\left(-7.25\right)^2\left(-2.75\right)^2 + 2\left(-7.25\right)^2\left(2.75\right)^2 \\
&+ 2\left(-7.25\right)^2\left(-2.75\right)^2 + 2\left(-7.25\right)^2\left(2.75\right)^2 \\
&+ 2\left(-1.25\right)^2\left(-2.75\right)^2 + 2\left(-1.25\right)^2\left(2.75\right)^2 \\
&+ 2\left(-1.25\right)^2\left(-2.75\right)^2 + 2\left(-1.25\right)^2\left(2.75\right)^2 \\
&+ 2\left(8.5\right)^2\left(-2.75\right)^2 + 2\left(8.5\right)^2\left(2.75\right)^2 \\
&+ 2\left(8.5\right)^2\left(-2.75\right)^2 + 2\left(8.5\right)^2\left(2.75\right)^2 \\
&= 7645.6875,
\end{aligned}
$$

$$
\begin{aligned}
&3\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)^2\\
&=3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2\\
&+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2\\
&+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2\\
&+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2\\
&+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+3\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2\\
&+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+3\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2\\
&=3\left(-1.91\overline{6}\right)^2(-2.75)^2+3\left(-1.91\overline{6}\right)^2(2.75)^2\\
&+3\left(1.91\overline{6}\right)^2(-2.75)^2+3\left(1.91\overline{6}\right)^2(2.75)^2\\
&+3\left(-1.91\overline{6}\right)^2(-2.75)^2+3\left(-1.91\overline{6}\right)^2(2.75)^2\\
&+3\left(1.91\overline{6}\right)^2(-2.75)^2+3\left(1.91\overline{6}\right)^2(2.75)^2\\
&+3\left(-1.91\overline{6}\right)^2(-2.75)^2+3\left(-1.91\overline{6}\right)^2(2.75)^2\\
&+3\left(1.91\overline{6}\right)^2(-2.75)^2+3\left(1.91\overline{6}\right)^2(2.75)^2\\
&=1000.140625,
\end{aligned}
$$

$$\sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\left(\overline{Y}_{i..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..r}-\overline{Y}_{...}\right)^2$$

$$= \left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2$$

$$+ \left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+\left(\overline{Y}_{1..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2$$

$$+ \left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2$$

$$+ \left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+\left(\overline{Y}_{2..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2$$

$$+ \left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.1.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2$$

$$+ \left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..1}-\overline{Y}_{...}\right)^2+\left(\overline{Y}_{3..}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{.2.}-\overline{Y}_{...}\right)^2\left(\overline{Y}_{..2}-\overline{Y}_{...}\right)^2$$

$$= (-7.25)^2\left(-1.91\overline{6}\right)^2(-2.75)^2+(-7.25)^2\left(-1.91\overline{6}\right)^2(2.75)^2$$

$$+ (-7.25)^2\left(1.91\overline{6}\right)^2(-2.75)^2+(-7.25)^2\left(1.91\overline{6}\right)^2(2.75)^2$$

$$+ (-1.25)^2\left(-1.91\overline{6}\right)^2(-2.75)^2+(-1.25)^2\left(-1.91\overline{6}\right)^2(2.75)^2$$

$$+ (-1.25)^2\left(1.91\overline{6}\right)^2(-2.75)^2+(-1.25)^2\left(1.91\overline{6}\right)^2(2.75)^2$$

$$+ (8.5)^2\left(-1.91\overline{6}\right)^2(-2.75)^2+(8.5)^2\left(-1.91\overline{6}\right)^2(2.75)^2$$

$$+ (8.5)^2\left(1.91\overline{6}\right)^2(-2.75)^2+(8.5)^2\left(1.91\overline{6}\right)^2(2.75)^2$$

$$= 14043.64128.$$

Thus, we have

$$\begin{aligned}
\widehat{\lambda}_{12} &= \frac{88.16666676}{3714.020834} = 0.02373887242,\\
\widehat{\lambda}_{13} &= \frac{379.5}{7645.6875} = 0.04963582412,\\
\widehat{\lambda}_{23} &= \frac{79.06249999}{1000.140625} = 0.07905138339, \text{ and}\\
\widehat{\lambda}_{123} &= \frac{18.44791667}{14043.64128} = 0.001313613493.
\end{aligned}$$

It follows that the SST, SSA, SSB, and $SSAB^*$ are

$$
\begin{aligned}
SST &= \sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\left(Y_{ijr} - \overline{Y}_{...}\right)^2 = (-4 - 6.25)^2 + (-1 - 6.25)^2 \\
&+ (-1 - 6.25)^2 + (2 - 6.25)^2 + (1 - 6.25)^2 \\
&+ (3 - 6.25)^2 + (5 - 6.25)^2 + (11 - 6.25)^2 \\
&+ (9 - 6.25)^2 + (13 - 6.25)^2 + (16 - 6.25)^2 \\
&+ (21 - 6.25)^2 \\
&= 656.25, \\
SSA &= 4\sum_{i=1}^{3}\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2 = 4((-7.25)^2 + (-1.25)^2 + (8.5)^2) \\
&= 505.5, \\
SSB &= 6\sum_{j=1}^{2}\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2 = 6(\left(-1.91\overline{6}\right)^2 + \left(1.91\overline{6}\right)^2) \\
&= 44.08333335, \\
SSC &= 6\sum_{r=1}^{2}\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2 = 6((-2.75)^2 + (2.75)^2) \\
&= 90.75, \\
SSAB^* &= \sum_{i=1}^{3}\sum_{j=1}^{2}\widehat{\lambda}_{12}^2\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2 \\
&= (0.02373887242)^2\,(3714.020834/2) \\
&= 1.046488627, \\
SSAC^* &= \sum_{i=1}^{3}\sum_{r=1}^{2}\widehat{\lambda}_{13}^2\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2 \\
&= (0.04963582412)^2\,(7645.6875/2) \\
&= 9.418397627, \\
SSBC^* &= \sum_{j=1}^{2}\sum_{r=1}^{2}\widehat{\lambda}_{23}^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2 \\
&= (0.07905138339)^2\,(1000.140625/3) \\
&= 2.083333333, \\
SSABC^* &= \sum_{i=1}^{3}\sum_{j=1}^{2}\sum_{r=1}^{2}\widehat{\lambda}_{123}^2\left(\overline{Y}_{i..} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{.j.} - \overline{Y}_{...}\right)^2\left(\overline{Y}_{..r} - \overline{Y}_{...}\right)^2 \\
&= (0.001313613493)^2\,(14043.64128) \\
&= 0.02423343226.
\end{aligned}
$$

We then have

$$\begin{aligned} SSE^* &= SST - SSA - SSB - SSC - SSAB^* - SSAC^* - SSBC^* - SSABC^* \\ &= 656.25 - 505.5 - 44.08333335 - 90.75 - 1.046488627 \\ &- 9.418397627 - 2.083333333 - 0.02423343226 \\ &= 3.344213631. \end{aligned}$$

The associated mean squares are

$$\begin{aligned} MSA &= \frac{505.5}{3-1} = 252.75; \\ MSB &= \frac{44.08333335}{2-1} = 44.08333335; \\ MSC &= \frac{90.75}{2-1} = 90.75; \\ MSAB^* &= \frac{1.046488627}{1} = 1.046488627; \\ MSAC^* &= \frac{9.418397627}{1} = 9.418397627; \\ MSBC^* &= \frac{2.083333333}{1} = 2.083333333; \\ MSABC^* &= \frac{0.02423343226}{1} = 0.02423343226; \text{ and} \\ MSE^* &= \frac{3.344213631}{3} = 1.114737877. \end{aligned}$$

The observed value of F is

$$\begin{aligned}
F_A &= \frac{252.75}{1.114737877} = 226.734917, \\
F_B &= \frac{44.08333335}{1.114737877} = 39.54591861, \\
F_C &= \frac{90.75}{1.114737877} = 81.40927286, \\
F_{AB^*} &= \frac{1.046488627}{1.114737877} = 0.9387755172, \\
F_{AC^*} &= \frac{9.418397627}{1.114737877} = 8.44897964, \\
F_{BC^*} &= \frac{2.083333333}{1.114737877} = 1.868899744, \text{ and} \\
F_{ABC^*} &= \frac{0.02423343226}{1.114737877} = 0.02173913057.
\end{aligned}$$

We see that if $\lambda = 0$, then the probability of the random variable $F_{1,3}$ is greater than or equal to F_{AB^*} is

$$\begin{aligned}
P\left(F_{1,3} \geq F_{AB^*}\right) &= 1 - P\left(F_{1,3} < F_{AB^*}\right) \\
&= 1 - \text{FDist}\left(0.9387755172; 1, 3\right) = 0.4040611181, \\
P\left(F_{1,3} \geq F_{AC^*}\right) &= 1 - P\left(F_{1,3} < F_{AC^*}\right) \\
&= 1 - \text{FDist}\left(8.44897964; 1, 3\right) = 0.0621622665, \\
P\left(F_{1,3} \geq F_{BC^*}\right) &= 1 - P\left(F_{1,3} < F_{BC^*}\right) \\
&= 1 - \text{FDist}\left(1.868899744; 1, 3\right) = 0.2650273957, \text{ and} \\
P\left(F_{1,3} \geq F_{ABC^*}\right) &= 1 - P\left(F_{1,3} < F_{ABC^*}\right) \\
&= 1 - \text{FDist}\left(0.02173913057; 1, 3\right) = 0.8921348612.
\end{aligned}$$

These results suggest there is no two or three factor interaction.

For the full model, the design matrix for the full model and our data in vector form are

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & -1 & 1 & 0 & -1 & 0 & -1 & -1 & 0 \\ 1 & 1 & 0 & -1 & 1 & -1 & 0 & 1 & 0 & -1 & -1 & 0 \\ 1 & 1 & 0 & -1 & -1 & -1 & 0 & -1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & -1 & 0 & 1 & 0 & -1 & -1 & 0 & -1 \\ 1 & 0 & 1 & -1 & 1 & 0 & -1 & 0 & 1 & -1 & 0 & -1 \\ 1 & 0 & 1 & -1 & -1 & 0 & -1 & 0 & -1 & 1 & 0 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix} \text{ and } \mathbf{y} = \begin{bmatrix} -4 \\ -1 \\ -1 \\ 2 \\ 1 \\ 3 \\ 5 \\ 11 \\ 9 \\ 13 \\ 16 \\ 21 \end{bmatrix}.$$

The matrix P associated with $\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}$ is

$$\mathbf{P} = \begin{bmatrix} \frac{\sqrt{12}}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{12}}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{12}}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{12}}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & -\frac{\sqrt{2}}{4} \end{bmatrix}.$$

The least squares estimates for the main effects and interaction is given by

$$\widehat{\theta} = \left(\mathbf{X^T X}\right)^{-1} \mathbf{X^T y} = \begin{bmatrix} \frac{25}{4} \\ -\frac{29}{4} \\ -\frac{5}{4} \\ -\frac{11}{4} \\ -\frac{23}{12} \\ \frac{5}{4} \\ -\frac{1}{4} \\ \frac{5}{12} \\ -\frac{1}{12} \\ \frac{5}{12} \\ -\frac{5}{12} \\ \frac{7}{12} \end{bmatrix}$$

the contrasts of the main effects and interactions are

$$\theta^* = \mathbf{P}^{-1}\theta = \begin{bmatrix} 2\sqrt{3}\theta_1 \\ \sqrt{6}\left(\theta_2 + \theta_3\right) \\ \sqrt{2}\left(\theta_2 - \theta_3\right) \\ 2\sqrt{3}\theta_4 \\ 2\sqrt{3}\theta_5 \\ \sqrt{6}\left(\theta_6 + \theta_7\right) \\ \sqrt{2}\left(\theta_6 - \theta_7\right) \\ \sqrt{6}\left(\theta_8 + \theta_9\right) \\ \sqrt{2}\left(\theta_8 - \theta_9\right) \\ 2\sqrt{3}\theta_{10} \\ \sqrt{6}\left(\theta_{11} + \theta_{12}\right) \\ \sqrt{2}\left(\theta_{11} - \theta_{12}\right) \end{bmatrix}.$$

The coordinates of the random vector $\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta}$ of estimators of the vector θ^* of the contrast of the main effects and interactions are independent. The estimates for these contrasts are

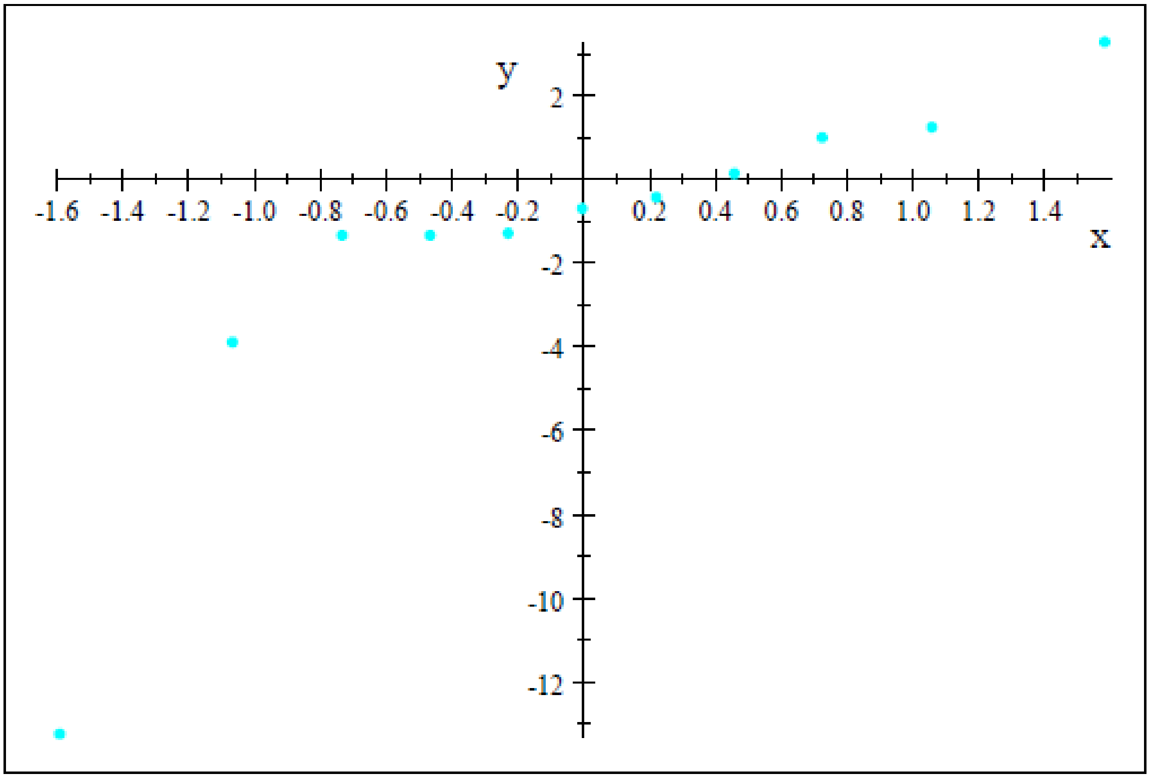
$$\widehat{\theta}^* = \mathbf{P}^{-1}\widehat{\theta} = \begin{bmatrix} 65.58699058 \\ -0.469485534 \\ -1.378858223 \\ -13.27905619 \\ -3.92598183 \\ 0.1020620726 \\ -1.378858223 \\ 1.204332457 \\ -0.7424621202 \\ 3.233161507 \\ -1.326806944 \\ 0.9545941546 \end{bmatrix}.$$

Removing the estimate $\widehat{\theta}_1^* = 65.58699058$, we have the 11×1 vector of ordered estimates of the given linear contrasts of the main effects and interactions along with the plotting positions for the corresponding normal probability plot given in the following 11×2 matrix.

$$\begin{bmatrix} -1.5864363519 & -13.27905619 \\ -1.0619165201 & -3.92598183 \\ -0.7288394047 & -1.378858223 \\ -0.4619783072 & -1.378858223 \\ -0.2248908792 & -1.326806944 \\ 0 & -0.7424621202 \\ 0.2248908792 & -0.469485534 \\ 0.4619783072 & 0.1020620726 \\ 0.7288394047 & 0.9545941546 \\ 1.0619165201 & 1.204332457 \\ 1.5864363519 & 3.233161507 \end{bmatrix}.$$

A plot of these points is given in the following figure.

Figure 3.1: Montgomery Example, Probability Plot

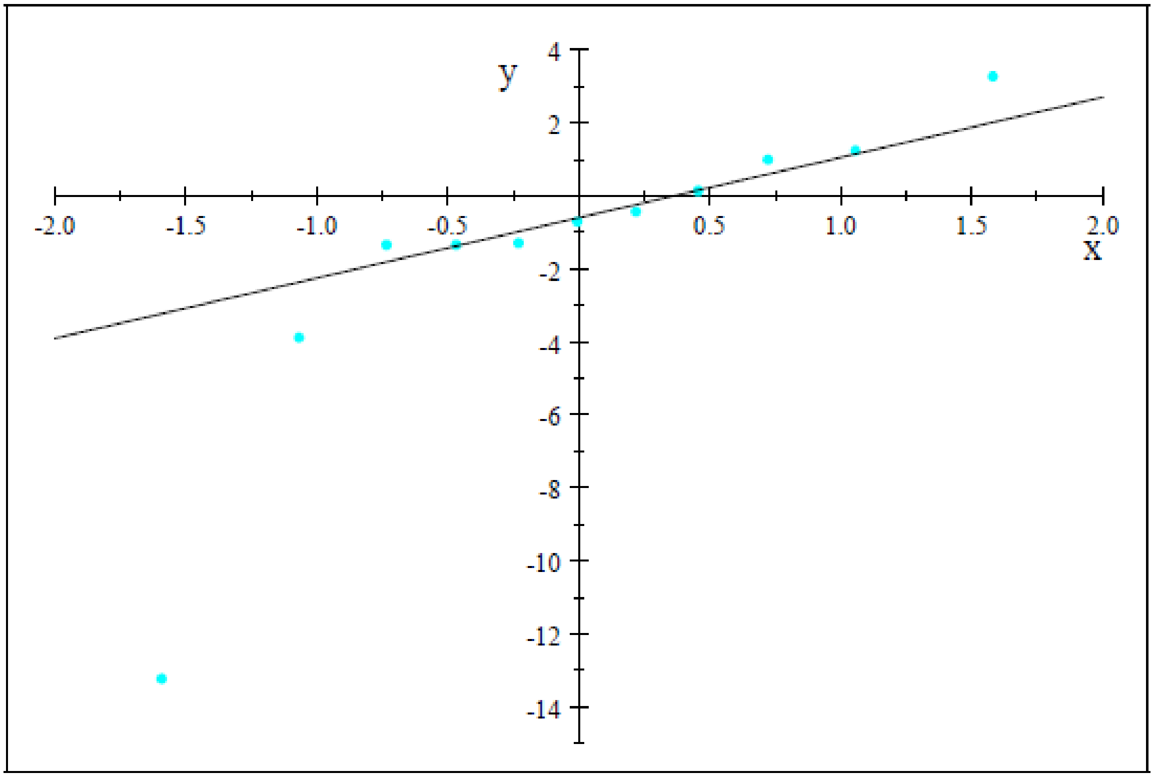


All the points seem to be plotting about a line except for the points with coordinates $(-1.5864363519, -13.27905619)$, $(-1.0619165201, -3.92598183)$ and $(1.5864363519, 3.233161507)$. Using the other eight points, we estimate the line to be

$$y = -0.5988288457 + 1.652812036x$$

A plot of this line along with our normal probability plot of the data is shown in the following figure.

Figure 3.2: Montgomery Example, Probability Plot and Fitted Line 8 Points



The contrast associated with the three estimates

$$\widehat{\theta}_4^*,\ \widehat{\theta}_5^*, \text{ and } \widehat{\theta}_{10}^*$$

are, respectively,

$$2\sqrt{3}\theta_4,\ 2\sqrt{3}\theta_5, \text{ and } 2\sqrt{3}\theta_{10}.$$

These contrast are associated with Factor B, Factor C and the interaction between Factor B and C. The plot shows no evidence there is an effect due to Factor A or interactions between Factors A and B, Factors A and C, and Factor A, B and C.

3.7 Conclusion

The method presented by Tukey (1949) was extended to the case of three factors. A method based on contrasts was also illustrated. This method can identify, as in the analysis of the a two factor experiment, contrasts of the main effects and/or interactions that are significantly different from zero.

CHAPTER 4

UNREPLICATED MULTIVARIATE FACTORIAL DESIGNS

4.1 Introduction

Multivariate analysis of variance (MANOVA) is commonly used in the analysis of factorial designs in which the response is a multivariate observation and there is a replicate for at least one treatment. For the case in which there is only one replicate per treatment, few if any methods have been developed for analyzing the data for one of these designs. The models for these designs are multivariate versions of the univariate designs. The main effects and interaction are now represented by vectors of parameters. In the next section, we will discuss these models. We follow this by a section that extends the method of Tukey (1949) for the unreplicated two factor experiment. This is followed by a section that discusses the use of multivariate contrasts to analysis the data from a factorial design. This is followed by a section which gives an example.

4.2 Design and Data Models

The additive model for a two factor experiment with no replicates. The response is a $p \times 1$ vector $\mathbf{Y}_{ij}$ of responses. Using an additive model, the response vector can be expressed

$$\mathbf{Y}_{ij} = \mu_{ij} + \epsilon_{ij}$$

with

$$\mu_{ij} = \mu + (\tau_1)_i + (\tau_2)_j + (\tau_{12})_{ij}$$

for $i = 1, \ldots, a$ and $j = 1, \ldots, b$. We have expressed the mean vector μ_{ij} of the response variable $\mathbf{Y}_{ij}$ as the sum of an overall mean vector μ, the vector of effects

$(\tau_1)_i$ due to setting the first factor at level i, the vector of effects $(\tau_2)_j$ of setting the second factor at its jth level, and a vector of effects $(\tau_{12})_{ij}$ due to the interaction between the two factors when the first is set at its ith level and the second at its jth level. It is assumed that

$$\sum_{i=1}^{a} (\tau_1)_i = 0;\ \sum_{j=1}^{b} (\tau_2)_j = 0;$$
$$\sum_{i=1}^{a} (\tau_{12})_{ij} = 0 \text{ for } j = 1, \ldots, b; \text{ and}$$
$$\sum_{j=1}^{b} (\tau_{12})_{ij} = 0 \text{ for } i = 1, \ldots, a.$$

We also assume that the $\mathbf{Y}_{ij}$'s are independent and $\epsilon_{ij} \sim N_p(\mathbf{0}, \mathbf{\Sigma})$ with $\mathbf{\Sigma}$ a positive definite matrix. Further, we assume that $ab > p$. We can express our model in matrix form as

$$\mathbf{Y} = \mathbf{X\Theta} + \epsilon,$$

where $\mathbf{X}$ is the design matrix used when $p = 1$,

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_{11}^{\mathbf{T}} \\ \mathbf{Y}_{12}^{\mathbf{T}} \\ \vdots \\ \mathbf{Y}_{ab}^{\mathbf{T}} \end{bmatrix}, \mathbf{\Theta} = \begin{bmatrix} \mu^{\mathbf{T}} \\ (\tau_1)_1^{\mathbf{T}} \\ \vdots \\ (\tau_{12})_m^{\mathbf{T}} \end{bmatrix} = \begin{bmatrix} \theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \\ \vdots & \vdots \\ \theta_{,1} & \theta_{m,2} \end{bmatrix}, \text{ and } \epsilon = \begin{bmatrix} \epsilon_{11}^{\mathbf{T}} \\ \epsilon_{12}^{\mathbf{T}} \\ \vdots \\ \epsilon_{ab}^{\mathbf{T}} \end{bmatrix},$$

where $m = (a-1)(b-1)$.

The additive model for a three factor experiment with no replicates express the $p \times 1$ response vector $\mathbf{Y}_{ijr}$ as

$$\mathbf{Y}_{ijr} = \mu + (\tau_1)_i + (\tau_2)_j + (\tau_3)_r + (\tau_{12})_{ij} + (\tau_{13})_{ir} + (\tau_{23})_{jr} + (\tau_{123})_{ijr} + \epsilon_{ijr},$$

where μ is the overall mean vector, $(\tau_1)_i$ main effect vector due to factor 1 set to level i, $(\tau_2)_j$ main effect vector due to factor 2 set to level j, $(\tau_3)_r$ main effect vector due to factor 3 set to level r, $(\tau_{12})_{ij}$, $(\tau_{13})_{ir}$, $(\tau_{23})_{jr}$ are the vectors associated with the two factor interactions, and $(\tau_{123})_{ijr}$'s are the vectors associated with the three factor interactions. It is assumed that ϵ_{ijr}'s are independent with a common $N_p(\mathbf{0}, \mathbf{\Sigma})$ distribution. Further, it is assumed that

$$\sum\nolimits_{i=1}^{a} (\tau_1)_i = 0;\ \sum\nolimits_{j=1}^{b} (\tau_2)_j = 0;\ \sum\nolimits_{r=1}^{c} (\tau_3)_r = 0;$$
$$\sum\nolimits_{j=1}^{b} (\tau_{12})_{ij} = 0 \text{ for } i = 1, \ldots, a;\ \sum\nolimits_{i=1}^{a} (\tau_{12})_{ij} = 0 \text{ for } j = 1, \ldots, b;$$
$$\sum\nolimits_{r=1}^{c} (\tau_{13})_{ir} = 0 \text{ for } i = 1, \ldots, a;\ \sum\nolimits_{i=1}^{a} (\tau_{13})_{ir} = 0 \text{ for } r = 1, \ldots, c;$$
$$\sum\nolimits_{r=1}^{c} (\tau_{23})_{jr} = 0 \text{ for } j = 1, \ldots, b;\ \sum\nolimits_{j=1}^{b} (\tau_{23})_{jr} = 0 \text{ for } r = 1, \ldots, c;$$
$$\sum\nolimits_{r=1}^{c} (\tau_{123})_{ijr} = 0 \text{ for } i = 1, \ldots, a,\ j = 1, \ldots, b;$$
$$\sum\nolimits_{j=1}^{b} (\tau_{123})_{ijr} = 0 \text{ for } i = 1, \ldots, a,\ r = 1, \ldots, c; \text{ and}$$
$$\sum\nolimits_{i=1}^{a} (\tau_{123})_{ijr} = 0 \text{ for } j = 1, \ldots, b,\ r = 1, \ldots, c.$$

We can express our model in matrix form as

$$\mathbf{Y} = \mathbf{X\Theta} + \epsilon,$$

where $\mathbf{X}$ is the design matrix used when $p = 1$,

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_{111}^{\mathbf{T}} \\ \mathbf{Y}_{112}^{\mathbf{T}} \\ \vdots \\ \mathbf{Y}_{abc}^{\mathbf{T}} \end{bmatrix},\ \mathbf{\Theta} = \begin{bmatrix} \mu^{\mathbf{T}} \\ (\tau_1)_1^{\mathbf{T}} \\ \vdots \\ (\tau_{123})_m^{\mathbf{T}} \end{bmatrix} = \begin{bmatrix} \theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \\ \vdots & \vdots \\ \theta_{m,1} & \theta_{m,2} \end{bmatrix},\ \text{and } \epsilon = \begin{bmatrix} \epsilon_{111}^{\mathbf{T}} \\ \epsilon_{112}^{\mathbf{T}} \\ \vdots \\ \epsilon_{abc}^{\mathbf{T}} \end{bmatrix},$$

where $m = (a-1)(b-1)(c-1)$. It is easy now to see that these models can be extended for more than three factors. However, the number of parameters in the model dramatically increase as the number of factors increases.

4.3 Parameter Estimation and Contrasts

The method of least squares can be used to estimate the parameters of the model. We have

$$\widehat{\boldsymbol{\Theta}} = \left(\mathbf{X^T X}\right)^{-1} \mathbf{X^T Y}.$$

Independent estimators $\widehat{\boldsymbol{\Theta}}^* = \mathbf{P}^{-1}\widehat{\boldsymbol{\Theta}}$ of the vector contrast $\boldsymbol{\Theta}^* = \mathbf{P}^{-1}\boldsymbol{\Theta}$ can be obtained using the $\mathbf{P}$ such that

$$\left(\mathbf{X^T X}\right)^{-1} = \mathbf{P P^T}.$$

This is the same $\mathbf{P}$ in the corresponding design in which the response is a univariate.

Separate normal probability plots of each column $\widehat{\boldsymbol{\Theta}}^*$ omitting the estimate corresponding to the overall mean can be constructed. One could then make a judgement about not only which of the main effects contrasts and interaction contrasts are significant but also which of these vectors are different from zero.

4.4 Example

Johnson and Wichern (2007) give on page 340 the following data for a two factor design without replicates.

Table 4.1: Johnson 's Example

		Factor 2			
		Level 1	Level 2	Level 3	Level 4
	Level 1	[6 8]'	[4 6]'	[8 12]'	[2 6]'
Factor 1	Level 2	[3 8]'	[-3 2]'	[4 3]'	[-4 3]'
	Level 3	[-3 3]'	[-4 5]'	[3 -3]'	[-4 -6]'

The design and data matrices are given, respectively, by

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & -1 & -1 & -1 & 0 & 0 & 0 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & -1 \\ 1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \text{ and } \mathbf{Y} = \begin{bmatrix} 6 & 8 \\ 4 & 6 \\ 8 & 12 \\ 2 & 6 \\ 3 & 8 \\ -3 & 2 \\ 4 & 3 \\ -4 & 3 \\ -3 & 2 \\ -4 & -5 \\ 3 & -3 \\ -4 & -6 \end{bmatrix}.$$

This is the same design matrix for a two factor experiment for the full additive model in which $a = 3$ and $b = 4$.

The least squares estimates for the parameters of the model are

$$\widehat{\boldsymbol{\Theta}} = \left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{Y} = \begin{bmatrix} 1 & 3 \\ 4 & 5 \\ -1 & 1 \\ 1 & 3 \\ -2 & -2 \\ 4 & 1 \\ 0 & -3 \\ 1 & 0 \\ -1 & 3 \\ 2 & 1 \\ -1 & 0 \\ 0 & -2 \end{bmatrix}.$$

Recall that the matrix $\mathbf{P}^{-1}$ associated with $\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1}$ is

$$\mathbf{P}^{-1} = \begin{bmatrix}
2\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \sqrt{6} & \sqrt{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{\sqrt{6}}{2} & 0 & -\frac{\sqrt{6}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{\sqrt{2}}{2} & -\sqrt{2} & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \sqrt{2} & \sqrt{2} & \sqrt{2} & \sqrt{2} & \sqrt{2} & \sqrt{2} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{3} & -\frac{\sqrt{6}}{3} & -\frac{\sqrt{6}}{3} & -\frac{\sqrt{6}}{3} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 & -\frac{\sqrt{3}}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & -1 & \frac{1}{2} & \frac{1}{2} & -1 & \frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6}
\end{bmatrix}.$$

The jth column of the matrix of contrasts $\mathbf{\Theta}^* = \mathbf{P}^{-1}\mathbf{\Theta}$ that are to be estimated by

$\widehat{\boldsymbol{\Theta}}^* = \mathbf{P}^{-1}\widehat{\boldsymbol{\Theta}}$ is

$$\begin{bmatrix} 2\sqrt{3}\theta_{1,j} \\ \sqrt{6}\left(\theta_{2,j}+\theta_{3,j}\right) \\ \sqrt{2}\left(\theta_{2,j}-\theta_{3,j}\right) \\ 2\left(\theta_{4,j}+\theta_{5,j}+\theta_{6,j}\right) \\ \frac{\sqrt{6}}{2}\left(\theta_{4,j}-\theta_{6,j}\right) \\ \frac{\sqrt{2}}{2}\left(\theta_{4,j}-2\theta_{5,j}+\theta_{6,j}\right) \\ \sqrt{2}\left(\theta_{7,j}+\theta_{8,j}+\theta_{9,j}+\theta_{10,j}+\theta_{11,j}+\theta_{12,j}\right) \\ \frac{\sqrt{6}}{3}\left(\theta_{7,j}+\theta_{8,j}+\theta_{9,j}-\theta_{10,j}-\theta_{11,j}-\theta_{12,j}\right) \\ \frac{\sqrt{3}}{2}\left(\theta_{7,j}-\theta_{9,j}+\theta_{10,j}-\theta_{12,j}\right) \\ \frac{1}{2}\left(\theta_{7,j}-2\theta_{8,j}+\theta_{9,j}+\theta_{10,j}-2\theta_{11,j}+\theta_{12,j}\right) \\ \frac{1}{2}\left(\theta_{7,j}-\theta_{9,j}-\theta_{10,j}+\theta_{12,j}\right) \\ \frac{\sqrt{3}}{6}\left(\theta_{7,j}-2\theta_{8,j}+\theta_{9,j}-\theta_{10,j}+2\theta_{11,j}-\theta_{12,j}\right) \end{bmatrix},$$

where the jth column of $\boldsymbol{\Theta}$ is

$$\begin{bmatrix} \theta_{1,j} \\ \theta_{2,j} \\ \theta_{3,j} \\ \theta_{4,j} \\ \theta_{5,j} \\ \theta_{6,j} \\ \theta_{7,j} \\ \theta_{8,j} \\ \theta_{9,j} \\ \theta_{10,j} \\ \theta_{11,j} \\ \theta_{12,j} \end{bmatrix}$$

for $j = 1, \ldots, p$.

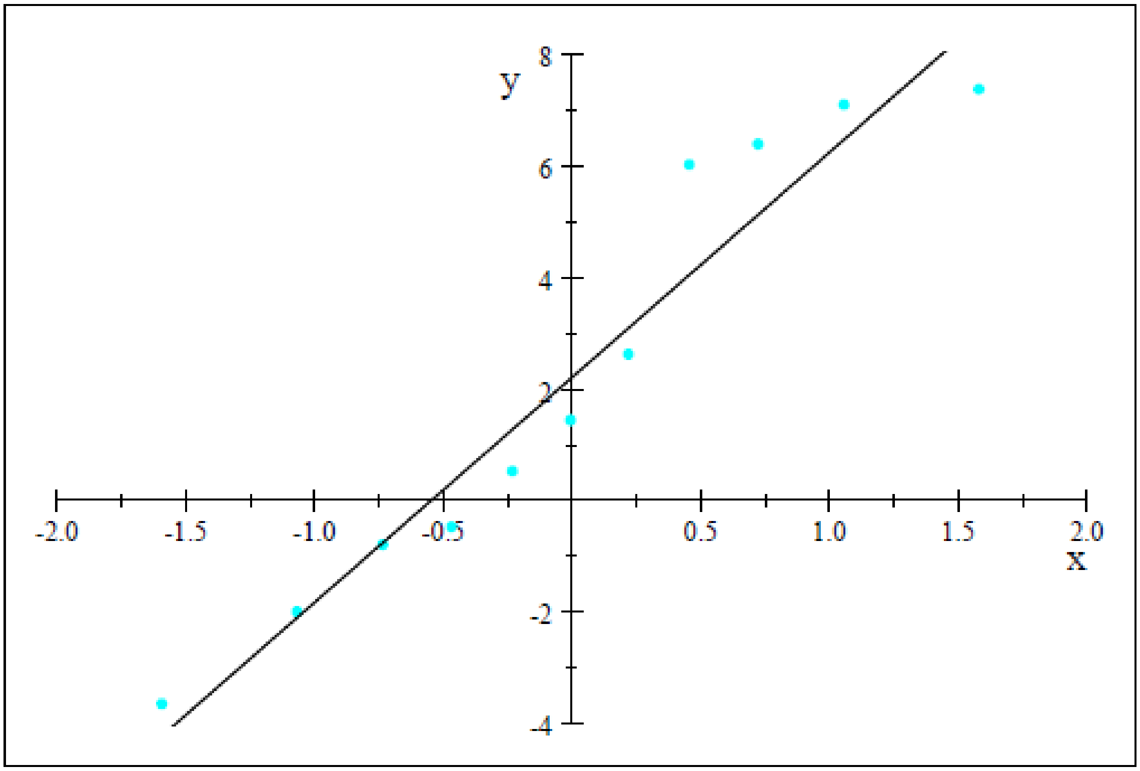
$$\widehat{\mathbf{\Theta}}^* = \begin{bmatrix} \widehat{\theta}_1^* & \widehat{\theta}_2^* \end{bmatrix} = \begin{bmatrix} 2\sqrt{3} & 6\sqrt{3} \\ 3\sqrt{6} & 6\sqrt{6} \\ 5\sqrt{2} & 4\sqrt{2} \\ 6 & 4 \\ -\frac{3}{2}\sqrt{6} & \sqrt{6} \\ \frac{9}{2}\sqrt{2} & 4\sqrt{2} \\ \sqrt{2} & -\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & \frac{1}{3}\sqrt{6} \\ \frac{3}{2}\sqrt{3} & -\frac{3}{2}\sqrt{3} \\ \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{9}{2} \\ -\frac{7}{6}\sqrt{3} & \frac{1}{6}\sqrt{3} \end{bmatrix} = \begin{bmatrix} 3.464101615 & 10.39230485 \\ 7.348469228 & 14.69693846 \\ 7.071067812 & 5.656854249 \\ 6.0 & 4.0 \\ -3.674234614 & 2.449489743 \\ 6.363961031 & 5.656854249 \\ 1.414213562 & -1.414213562 \\ -0.8164965809 & 0.8164965809 \\ 2.598076211 & -2.598076211 \\ 0.5 & -0.5 \\ -0.5 & -4.5 \\ -2.020725942 & 0.2886751346 \end{bmatrix}.$$

The coordinates of the random vector $\widehat{\mathbf{\Theta}}^*$of estimators of the vector $\mathbf{\Theta}^*$ of the contrast of the main effects and interactions are independent. The ordered estimates for these contrasts and the associated contrasts are given in the following table.

$$\begin{bmatrix} -3.674234614 & \frac{\sqrt{6}}{2}\left(\theta_{4,1}-\theta_{6,1}\right) \\ -2.020725942 & \frac{\sqrt{3}}{6}\left(\theta_{7,1}-2\theta_{8,1}+\theta_{9,1}-\theta_{10,1}+2\theta_{11,1}-\theta_{12,1}\right) \\ -0.8164965809 & \frac{\sqrt{6}}{3}\left(\theta_{7,1}+\theta_{8,1}+\theta_{9,1}-\theta_{10,1}-\theta_{11,1}-\theta_{12,1}\right) \\ -0.5 & \frac{1}{2}\left(\theta_{7,1}-\theta_{9,1}-\theta_{10,1}+\theta_{12,1}\right) \\ 0.5 & \frac{1}{2}\left(\theta_{7,1}-2\theta_{8,1}+\theta_{9,1}+\theta_{10,1}-2\theta_{11,1}+\theta_{12,1}\right) \\ 1.414213562 & \sqrt{2}\left(\theta_{7,1}+\theta_{8,1}+\theta_{9,1}+\theta_{10,1}+\theta_{11,1}+\theta_{12,1}\right) \\ 2.598076211 & \frac{\sqrt{3}}{2}\left(\theta_{7,1}-\theta_{9,1}+\theta_{10,1}-\theta_{12,1}\right) \\ 6.0 & 2\left(\theta_{4,1}+\theta_{5,1}+\theta_{6,1}\right) \\ 6.363961031 & \frac{\sqrt{2}}{2}\left(\theta_{4,1}-2\theta_{5,1}+\theta_{6,1}\right) \\ 7.071067812 & \sqrt{2}\left(\theta_{2,1}-\theta_{3,1}\right) \\ 7.348469228 & \sqrt{6}\left(\theta_{2,1}+\theta_{3,1}\right) \end{bmatrix}.$$

Normal probability plots of the estimated contrasts of the main effects and interactions are given in the Figure 4.1.

Figure 4.1: Johnson Example, Probability Plot 1



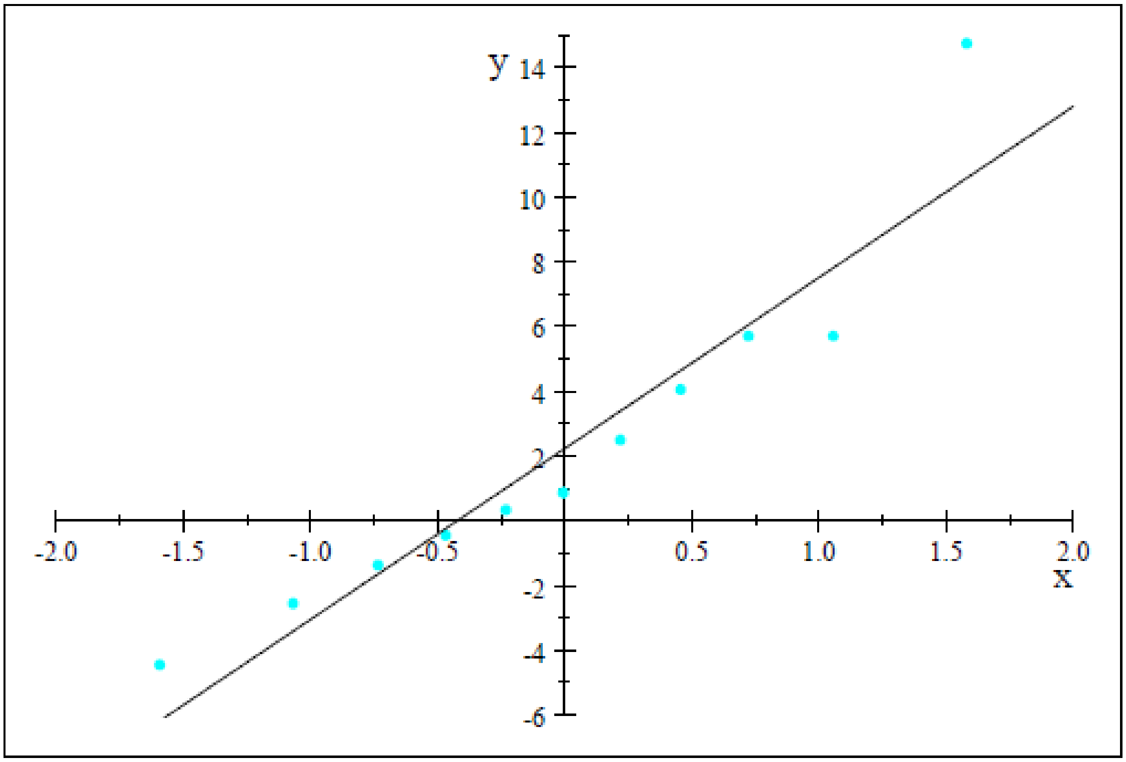
It appears that there are two outliers whose coordinates are $(0.4619783, 6.0)$ and $(0.7288394, 6.363961)$. The second coordinates of these two points are estimates of the respective contrasts

$$2\left(\theta_{4,1} + \theta_{5,1} + \theta_{6,1}\right) \text{ and } \frac{\sqrt{2}}{2}\left(\theta_{4,1} - 2\theta_{5,1} + \theta_{6,1}\right).$$

Thus, we would conclude that relative to the first response variable, the only effect is due to the second factor.

A normal probability plot of the estimates of the contrasts associate with the main effects and interactions associated with the second response variable is given in the following figure.

Figure 4.2: Johnson Example, Probability Plot 2



It appears that the point with coordinates $(1.5864363519, 14.69693846)$ is the only point associated with a contrast that is not zero. This contrast is the parameter $\sqrt{6}\,(\theta_{2,2} + \theta_{3,2})$ which is associated with the first factor. We conclude that there are effects due to both the factors but there is no interaction between the factors.

4.5 Conclusion

We have shown that our contrast method can be used with unreplicated factorial designs in which the response variable is a multivariate set of measurements. Some illustrative examples were given.

CHAPTER 5

CONCLUSION

5.1 General Conclusions

In this paper, we consider factorical design models with univariate and multivariate responses. Under univariate case, methods for analyszing data from two factor and three factor unreplicated designs were examined. For the two factor design model, we first looked at the method for analyzing a full model with replicates and a reduced model without replicates. For the full model without replicates we considered Tukey's method to test for non-additivity for a two factor experiment. We extended Tukey's method for non-additivity to the case of three factors. Some examples were given. Our method was extended to k factor experiments in which the response is a multivariate set of measurements.

5.2 Areas for Further Research

We are interested in investigating the following topic areas for k factorial designs without replicates.

(1) The method of Tukey (1949) extended for more than two factors for a univariate response.

(2) The method of Tukey (1949) extended for two or more factors for a multivariate response.

(3) Examining methods for analyzing the data from an unreplicated two level factor designs with a multivariate response. These methods include separate normal probability plots for the estimated main effects and interactions for each component of the response variable. Also, we are interested in examining various orderings of

the vectors of statistics that are used to estimate the vector valued main effects and interactions.

(4) To make the use of our results more readily available to the research, we plan to develop software to implement these methods.

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